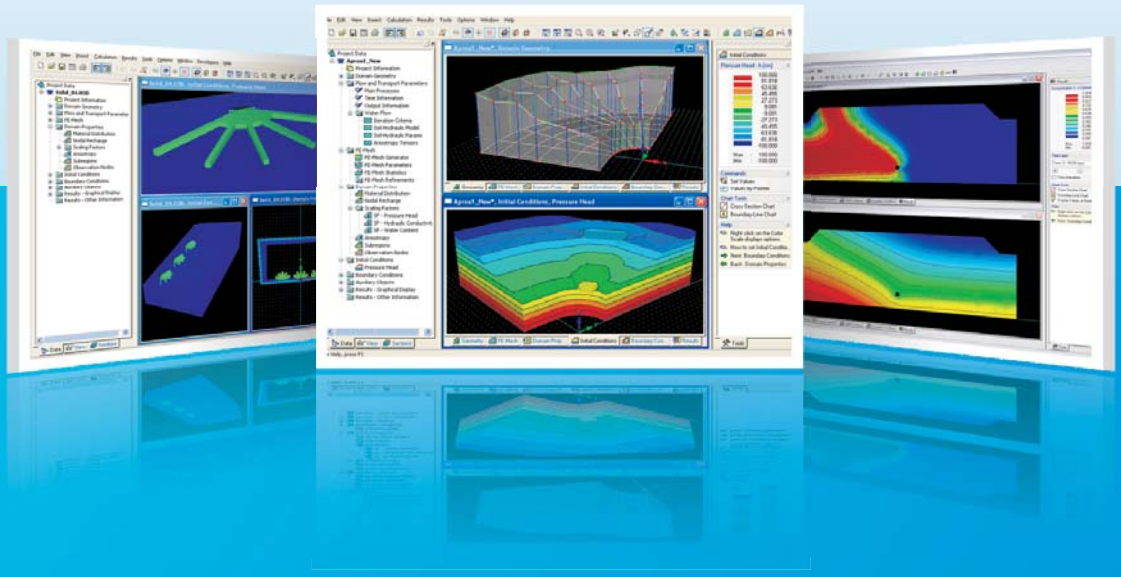
PC-PROGRESS
Engineering software developer

HYDRUS

User Manual
Version 2



Software Package for Simulating the Two- and Three-Dimensional Movement of Water, Heat and Multiple Solutes in Variably-Saturated Media

January 2011, PC-Progress, Prague, Czech Republic
© 2011 J.šimůnek and M. Šejna. All rights reserved

The HYDRUS Software Package for Simulating the Two- and Three-Dimensional Movement of Water, Heat, and Multiple Solutes in Variably-Saturated Media

User Manual

Version 2

M. Šejna[1], J. Šimůnek[2], and M. Th. van Genuchten[3]

May 2011

[1]PC-Progress, Prague, Czech Republic
[2]University of California Riverside, Riverside, CA
[3]Department of Mechanical Engineering, Federal University of Rio de Janeiro, Brazil

© 2011 J. Šimůnek and M. Šejna. All rights reserved.

Table of Contents

Table of Contents 3
List of Figures 9
List of Tables 17
Abstract 19
Introduction to the HYDRUS Graphical User Interface 23
1. **Project Manager and Data Management** 27
2. **Projects Geometry Information** 33
3. **Flow Parameters** 39
   3.1. *Main Processes* 39
   3.2. *Inverse Solution* 40
   3.3. *Time Information* 44
   3.4. *Output Information* 46
   3.5. *Iteration Criteria* 48
   3.6. *Soil Hydraulic Model* 51
   3.7. *Water Flow Parameters* 53
   3.8. *Neural Network Predictions* 57
   3.9. *Anisotropy in the Hydraulic Conductivity* 58
   3.10. *Solute Transport* 59
   3.11. *Solute Transport Parameters* 64
   3.12. *Solute Reaction Parameters* 65
   3.13. *Temperature Dependence of Solute Transport Parameters* 69
   3.14. *Water Content Dependence of Solute Transport Parameters* 70
   3.15. *Solution Compositions for the UNSATCHEM Module* 71
   3.16. *Chemical Parameters for the UNSATCHEM Module* 72
   3.17. *Heat Transport Parameters* 73
   3.18. *Root Water Uptake Model* 75
   3.19. *Root Water Uptake Parameters* 77
   3.20. *Root Distribution Parameters* 80
   3.21. *Time Variable Boundary Conditions* 82
   3.22. *Constructed Wetlands* 84
4. **Geometry of the Transport Domain** 95

4.1. *Boundary Objects* 95
4.1.1. *Points* 98
4.1.2. *Lines and Polylines* 101
4.1.3. *Arcs and Circles* 102
4.1.4. *Curves and Splines* 105
4.1.5. *Common Information for a Graphical Input of Objects* 107
4.1.6. *Translate, Copy, Rotate, Mirror, Stretch, and Skew Operations* 108
4.1.7. *Additional Operations* 110
4.2. *Surfaces* 111
4.2.1. *General Definitions.* 111
4.2.1.1. *Planar Surfaces* 113
4.2.1.2. *Curved Surfaces* 114
4.2.1.3. *Partial Surfaces* 116
4.2.2. *Steps to Define a Two-Dimensional Domain.* 116
4.2.3. *Several notes on rules for correct definition of the Geometry.* 117
4.2.4. *Internal Objects.* 118
4.2.5. *Check and Repair Geometry.* 121
4.3. *Openings* 114
4.4. *Solids* 123
4.4.1. *3D-Layered – Hexahedral Solids.* 123
4.4.2. *3D-Layered – General Solids.* 124
4.4.2.1. *Division of a Solid into Columns.* 128
4.4.2.2. *Division of a Solid into Geo-Layers.* 128
4.4.2.3. *Individual specification of different Thicknesses of Geo-Layers at different Thickness Vectors.* 128
4.4.2.4. *Steps to Define a 3D-Layered Domain.* 129
4.4.3. *3D-General Solids.* 129
4.5. *Thickness Vectors* 132
4.6. *Intersections of Surface and Solids* 136
4.7. *Auxiliary Objects* 136
4.7.1. *Dimensions* 138
4.7.2. *Labels* 139
4.7.3. *Bitmaps (Textures)* 140

4.7.4. *Cross-Sections* 141
4.7.5. *Mesh-Lines* 141
4.7.6. *Background Layers* 143
4.8. *Other Notes on Objects* 145
4.8.1. *Object Numbering* 145
4.8.2. *Relations among Objects* 145
4.8.3. *References among Objects and Convention for Writing a List of Indices* 145
4.9. *Import Geometry from a Text File* 145
4.10. *Import Geometry from a DXF File* 148
4.11. *Import Geometry from a TIN File* 148
5. **Finite Element Mesh** 149
5.1. *Finite Element Mesh Generator* 149
5.2. *Structured Finite Element Mesh Generator* 149
5.3. *Unstructured Finite Element Mesh Parameters* 152
5.4. *Finite Element Mesh Refinement* 158
5.4.1. *Finite Element Mesh Refinement for MeshGen2D* 158
5.4.2. *Finite Element Mesh Refinement for Genex/T3D* 161
5.5. *Unstructured Finite Element Mesh Generator MeshGen2D* 164
5.6. *Finite Element Mesh Statistics* 168
5.7. *Finite Element Mesh Sections* 169
6. **Domain Properties, Initial and Boundary Conditions** 171
6.1. *Default Domain Properties* 171
6.2. *Initial Conditions* 172
6.3. *Boundary Conditions* 175
6.3.1. *Time-Variable Head/Flux 1 BCs* 176
6.3.2. *Special Boundary Conditions* 177
6.3.3. *Triggered Irrigation* 180
6.4. *Domain Properties* 181
6.5. *Defining Properties on Geometrical Objects* 184
6.5.1. *Materials on Geometrical Objects* 186
6.5.2. *Observation Nodes on Geometrical Objects* 189
6.5.3. *Initial Conditions on Geometrical Objects* 190
6.5.4. *Boundary Conditions on Geometrical Objects* 191

6.5.5. *Additional Notes on Properties at Geometrical Objects* 192
7. **Graphical Output**.....193
7.1. *Results – Graphical Display* 193
7.1.1. *Displayed Variables*.....194
7.1.2. *Display Options* 199
7.1.3. *Edit Isoband Value and Color Spectra* 200
7.2. *Results – Other Information*.....206
7.2.1. *Convert to ASCII*.....209
8. **Graphical User Interface Components** 211
8.1. *View Window* 211
8.1.1 *Scene and Viewing Commands* 211
8.1.2 *Grid and Work Plane* 212
8.1.3 *Stretching Factors*.....213
8.1.4. *Rendering Model* 214
8.1.5. *Selection and Edit Commands* 214
8.1.6. *Pop-up Menus* 215
8.1.7. *Drag and Drop*.....216
8.1.8. *Sections* 216
8.2. *Navigator Bars*.....219
8.3. *Edit Bars* 221
8.4. *Toolbars* 226
8.5. *HYDRUS Menus*.....230
9. **Miscellaneous Information**.....251
9.1. *Program Options* 251
9.2. *HYDRUS License and Activation*.....255
9.2.1. *Brief Description of HYDRUS Activation*.....255
9.2.2. *Detailed Description of HYDRUS Activation*.....255
9.2.2.1. *On-Line Activation* 258
9.2.2.2. *Activation by E-mail*.....260
9.2.3. *Detailed Description of HYDRUS Activation*.....266
9.2.3.1. *On-Line Deactivation*.....267
9.2.3.2. *Deactivation by E-mail*.....268
9.2.4. *Extending Activation*.....269

9.3. *Print Options*.....270
9.4. *Print Preview and Copy to the Clipboard Commands*.....271
9.5. *Coordinate Systems*.....272
9.6. *DOS Window During Calculations*.....273
9.7. *Video Files*.....274
9.8. *About HYDRUS*.....276
References.....277

List of Figures

Figure 1. The HYDRUS Graphical User Interface (the main window). 24
Figure 2. The project Manager with the Project Groups tab. 27
Figure 3. The Project Manager with the Projects tab. 28
Figure 4. The Project Information dialog window. 30
Figure 5. General description of the HYDRUS Project Groups. 30
Figure 6. The Domain Type and Units dialog window (with 3D preview). 33
Figure 7. Domain Type and Units dialog window (with 2D axisymmetrical preview). 34
Figure 8. Examples of rectangular (top) and general (bottom) two-dimensional geometries. 35
Figure 9. Example of a hexahedral three-dimensional geometry. 36
Figure 10. The Rectangular Domain Definition dialog window. 36
Figure 11. The Hexahedral Domain Definition dialog window. 37
Figure 12. The Main Processes dialog window. 39
Figure 13. The Inverse Solution dialog window. 40
Figure 14. The Data for Inverse Solution dialog window. 41
Figure 15. The Time Information dialog window. 44
Figure 16. The Output Information dialog window. 46
Figure 17. The Iteration Criteria dialog window. 48
Figure 18. The Soil Hydraulic Model dialog window. 51
Figure 19. The Water Flow Parameters dialog window for direct (top) and inverse (bottom) problems. 53
Figure 20. The Rosetta Lite (Neural Network Predictions) dialog window. 57
Figure 21. The Edit Local Anisotropy dialog window for two-dimensional applications. 58
Figure 22. The Tensors of the Anisotropy dialog window 58
Figure 23. The Solute Transport dialog window. 59
Figure 24. The Solute Transport dialog window for the UNSATCHEM module. 63
Figure 25. The Solute Transport Parameters dialog window. 64
Figure 26. The Solute Reaction Parameters dialog window. 65
Figure 27. The Solute Reaction Parameters dialog window for the UNSATCHEM module. 68
Figure 28. The Temperature Dependent Solute Transport and Reaction Parameters dialog window. 69
Figure 29. The Water Content Dependent Solute Reaction Parameters dialog window. 70

Figure 30. The Solution Compositions dialog window for the UNSATCHEM module. 71
Figure 31. The Chemical Parameters dialog window for the UNSATCHEM module. 72
Figure 32. The Heat Transport Parameters dialog window.....73
Figure 33. The Root Water Uptake Model dialog window. 75
Figure 34. The Root Water Uptake Parameters dialog window for the stress response function of *Feddes* et al. [1978] (left) and *van Genuchten* [1985] (right). 77
Figure 35. The Root Water Uptake Parameters dialog window for the solute stress response function based on the threshold model (left) and S-shape model of *van Genuchten* [1985] (right).....78
Figure 36. The Root Distribution Parameters dialog window.....81
Figure 37. The Time Variable Boundary Conditions dialog window. 82
Figure 38. The Constructed Wetland Model (CW2D) Parameter I dialog window.....86
Figure 39. The Constructed Wetland Model (CWM1) Parameter I dialog window. 89
Figure 40. The Constructed Wetland Model (CW2D) Parameter II dialog window. 90
Figure 41. The Constructed Wetland Model (CWM1) Parameter II dialog window.....92
Figure 42. A base surface showing several basic geometric objects.....98
Figure 43. The Edit Bar during the process of defining graphically a new point (left) and a new line (right). 99
Figure 44. The Edit Point dialog window. 100
Figure 45. Different ways of adding Parametric Points on a curve. 101
Figure 46. The Edit Curve dialog window. 102
Figure 47. The Edit Bar during the process of defining graphically a radius for a new arc (left) or a new circle (right). 103
Figure 48. The New Line (Arc) dialog window. 104
Figure 49. The New Line (Circle) dialog window. 105
Figure 50. Edit Bar during the process of defining graphically a spline. 106
Figure 51. Snap to a point (left) and snap to a curve (right). 107
Figure 52. The Translate - Copy dialog windows. 108
Figure 53. The Rotate (left) and Mirror (right) dialog windows. 109
Figure 54. The Stretch (left) and Skew (right) dialog windows. 109
Figure 55. The Insert Point on Curve dialog window. 110
Figure 56. The warning issued when Surfaces cannot be created automatically and must be defined manually.....112
Figure 57. Edit Bar during the process of defining graphically a surface (left) and the General tab of the Edit Surface dialog window (right). 112

Figure 58. A solid showing the base surface. 113
Figure 59. Solid showing separate vertical columns. 113
Figure 60. A solid with its base surface in the XZ plane and thickness vectors in the Y direction. 114
Figure 61. FE-Mesh for a solid with its base surface in the XZ plane and thickness vectors in the Y direction 114
Figure 62. Examples of Curved Surfaces (Rotary, Pipe, B-Spline, and Quadrangle Surfaces). . 115
Figure 63. The Integrated Tab of the Edit Surface dialog window. 118
Figure 64. An example of internal objects. 119
Figure 65. An example of an Upper Surface definition using Internal Curves and Thickness Vectors. 120
Figure 66. The Repair Domain Definition dialog window. 121
Figure 67. The New Opening dialog window. 122
Figure 68. The Edit Bar during the process of graphically defining a Hexahedral Solid. Definition of a Base Surface on the left and a Thickness on the right 123
Figure 69. The Edit Bar during the process of graphically defining a Solid by extruding a Base Surface. Selection of a Surface (left) and definition of a Thickness Vector (right). . 124
Figure 70. The 3D-Layered Solid dialog window; the General, Geo-Layers, and Thickness Profiles Tabs. 126
Figure 71. The 3D-Layered Solid dialog window; the FE-Mesh Tab for single and multiple layers. 127
Figure 72. Examples of 3D-General Solids. Top - formed by Planar Surfaces, bottom – formed by curved surfaces 130
Figure 73. Edit Bar during the process of graphically defining a Thickness Vector. 133
Figure 74. The Thickness dialog window. 133
Figure 75. A solid with several thickness vectors. 134
Figure 76. FE-Mesh for the solid in Figure 75. 134
Figure 77. Missing internal curves in the base surface. 135
Figure 78. Consequence of missing an internal curve in the base surface on the FE-Mesh of the top surface. 135
Figure 79. The Edit Intersection dialog window (for two Surfaces (left) and two Solids (right). 136
Figure 80. An example of an Intersection of two Surfaces and a resulting Partial Surface and Intersection Curve. 137
Figure 81. Edit Bar during the process of graphically defining a Dimension. Selection of two definition points, the distance of which is to be labeled (left) and the dimension type (right). 138

Figure 82. The Edit Comment dialog window. 139
Figure 83. The Edit Bar during the process of graphically defining a Comment. Selection of the Comment Position, Comment Text, Font and Color (left) and Offset (right). 140
Figure 84. The Edit Bitmap dialog window. 140
Figure 85. The Cross-Section dialog window. 141
Figure 86. The Mesh-Line dialog window. 142
Figure 87. The Fluxes across Mesh-Line dialog window. 142
Figure 88. An example of the Background Layer. 143
Figure 89. The Import Geometry from a DXF File dialog window. 148
Figure 90. The Rectangular Domain Discretization dialog window. 150
Figure 91. The Hexahedral Domain Discretization dialog window. 151
Figure 92. The FE-Mesh Parameters dialog window (the Main Tab for 3D-Layered (left) and 3D-General (right) geometries). 152
Figure 93. The FE-Mesh Parameters dialog window (Tab Stretching). 153
Figure 94. The FE-Mesh Parameters dialog window (Tab MG Options). 154
Figure 95. The FE-Mesh Parameters dialog window (Tab Options). 156
Figure 96. The FE-Mesh Parameters dialog window (Mesh Section Tab). 157
Figure 97. The New FE-Mesh Refinement dialog window for the MeshGen2D module with four different types of refinements (applied to a Point, a Line with a given FE-size or the number of Points, and to a Surface). 159
Figure 98. Example of FE-Mesh Refinements (top) and FE-Mesh (bottom). 123
Figure 99. Circular (left) and rectangular (right) refinements around a node. 161
Figure 100. Refinement on a line (by defining either the size or the number of finite elements along a line). 162
Figure 101. Refinements on a surface (left) or solid (right). 162
Figure 102. The FE-Mesh Refinement dialog window for the Genex/T3D module with six different types of refinements (applied to a Circular or a Rectangular Point, a Line with a given FE-size or a number of points, to a Surface, and to a Solid). 164
Figure 103. Example of mesh stretching using a stretching factor of 3 in the *x*-direction. 167
Figure 104. The FE-Mesh Information dialog window for a two-dimensional problem (top) and a three-dimensional problem (bottom). 168
Figure 105. The FE-Mesh Sections dialog window. 170
Figure 106. The Default Domain Properties dialog window. 172
Figure 107. The Water Flow Initial Condition dialog window. 173
Figure 108. The Temperature distribution dialog window. 174

Figure 109. The Import Initial Condition dialog window. 175
Figure 110. The Time-Variable Head/Flux 1 BCs tab of the Boundary Condition Options dialog window. 177
Figure 111. The Special Boundary Conditions tab of the Boundary Condition Options dialog window. 180
Figure 112. The Triggered Irrigation tab of the Boundary Condition Options dialog window. 181
Figure 113. The Stochastic Distribution of Scaling Factors dialog window. 182
Figure 114. The Stochastic Parameters dialog window. 183
Figure 115. An example of the transport domain defined using three components S1, S2, and S3. 184
Figure 116. The upper part of the Edit Bar, which displays defined materials and commands for various actions with materials. 186
Figure 117. The Set Materials dialog window. 187
Figure 118. The transport domain with materials specified on geometrical objects. 187
Figure 119. The Sort Property Objects dialog window. 188
Figure 120. The Edit Materials dialog window. 189
Figure 121. The Observation Node dialog window. 190
Figure 122. The Edit Pressure Head (left) and Concentration (right) Initial Conditions dialog window. 191
Figure 123. The Edit Water Flow Boundary Condition dialog window. 192
Figure 124. The "Results - Graphical Display" part of Data Tab of the Navigator Bar for the standard (left), Unsatchem (centre), and Wetland (right) modules. 197
Figure 125. The "Results" part of the View Tab of the Navigator Bar with the display of various alternative variables. 198
Figure 126. The Display Options dialog window. 199
Figure 127. The Edit Isoband Value and Color Spectra dialog window. 200
Figure 128. The use of intermediate isolines. 201
Figure 129. The Color dialog window. 202
Figure 130. Adjusting scale in the Edit Isoband Value and Color Spectra dialog window. 203
Figure 131. The use of the Custom Scale. 204
Figure 132. The color smoothing. 205
Figure 133. The Convert to ASCII dialog window. 209
Figure 134. *x-y* graph dialog window displaying pressure heads in observation nodes. 206
Figure 135. The Grid and Work Plane dialog window. 212
Figure 136. The View Stretching Factors dialog window. 213

Figure 137. The Rendering part of the View Tab of the Navigator Bar. 214
Figure 138. The Pop-up Menu from the View window. 216
Figure 139. Options for Generation of Geo-Sections and FE-Mesh Sections dialog window. .217
Figure 140. Selected Navigator Bars (Data Tabs on the left and in the middle, the View Tab on the right). 220
Figure 141. Selected Edit Bars (from left to right) for Material Distribution in Domain Properties, Water Flow Boundary Conditions, Pressure Head Initial Conditions, and Water Content Results. 221
Figure 142. The Color Scale Display Options menu.....225
Figure 143. Selected Edit Bars (for Domain Geometry and FE-Mesh). 225
Figure 144. The Toolbars dialog window. 226
Figure 145. The Customize Toolbars dialog window. 226
Figure 146. The HYDRUS Menus I (File, Edit, and View).....230
Figure 147. The HYDRUS Menus II (Insert, Calculations, and Results). 231
Figure 148. The HYDRUS Menus II (Tools, Options, Windows, and Help). 231
Figure 149. The Program Options dialog window (the Graphics Tab). 251
Figure 150. The Program Options dialog window (the Program Options Tab). 252
Figure 151. The FE-Mesh Options dialog window (the Program Options Tab). 253
Figure 152. The Program Options dialog window (the Files and Directories Tab). 254
Figure 153. The HYDRUS Authorization Status dialog window (Tab Status). 256
Figure 154. Warning issued when attempting to make changes to the Authorization Status while not running HYDRUS with administrator privileges.. 257
Figure 155. The HYDRUS Authorization Status dialog window (Tab Add-on Modules). 257
Figure 156. The HYDRUS License and Activation dialog window (Tab History of Activation). 258
Figure 157. The Online Activation dialog window. 259
Figure 158. Window requesting confirmation of entered parameters. 260
Figure 159. The Activation by E-mail dialog window (Tab Step 1). 271
Figure 160. The Activation by E-mail dialog window (Tab Step 2). 262
Figure 161. Email with the HYDRUS Activation Request in Outlook.....263
Figure 162. Window inquiring if the user wants to enter the Activation Code.....264
Figure 163. The Activation by E-mail dialog window (Tab Step 3). 265
Figure 164. Window confirming successful HYDRUS authorization. 265
Figure 165. Window reporting a failure of HYDRUS authorization. 266

Figure 166. The Online Deactivation dialog window. 267
Figure 167. Window confirming successful online deactivation of HYDRUS. 267
Figure 168. The HYDRUS Deactivation dialog window.....268
Figure 169. Window confirming successful deactivation of HYDRUS by email. 269
Figure 170. The General, Picture, and Legend tabs of the Print Options dialog window.....270
Figure 171. The Coordinate Systems dialog windows.....272
Figure 172. The Create Video File dialog window. 274
Figure 173. Result of commands Print Preview or Copy to the Clipboard.....271
Figure 174. The About HYDRUS dialog window (the Program tab (top) and the Authors tab (bottom).....276

List of Tables

Table 1. Commands in the Project Manager. 29

Table 2. Data types for the objective function (Inverse Problem). 42

Table 3. Definition of the column *X* in Fig. 14 based on Data Type (Inverse Problem). 42

Table 4. Definition of the column *Y* in Fig. 14 based on Data Type (Inverse Problem) 43

Table 5. Time Information variables. 45

Table 6. Time Step Control variables. 50

Table 7. Soil hydraulic parameters for the analytical functions of *van Genuchten* [1980] for twelve textural classes of the USDA soil textural triangle according to *Carsel and Parish* [1988]. 55

Table 8. Soil hydraulic parameters for the analytical functions of *van Genuchten* [1980] for twelve textural classes of the USDA textural triangle as obtained with the Rosetta Lite program [*Schaap et al.,* 2001]. 55

Table 9. Soil hydraulic parameters for the analytical functions of *Brooks and Corey* [1964] for twelve textural classes of the USDA soil textural triangle according to *Carsel and Parish* [1988]. 56

Table 10. Soil hydraulic parameters for the analytical functions of *Kosugi* [1996] for twelve textural classes of the USDA soil textural triangle. 56

Table 11. Comparison of CW2D and CWM1 components. 84

Table 12. Comparison of CW2D and CWM1 processes. 85

Table 13. Kinetic parameters in the CW2D biokinetic model [*Langergraber and Šimunek,* 2005]. 87

Table 14. Kinetic parameters in the CWM1 biokinetic model [*Langergraber et al.,* 2009]. 88

Table 15. Temperature dependences, stoichiometric parameters, composition parameters and parameters describing oxygen transfer in the CW2D biokinetic model [*Langergraber and Šimunek,* 2005]. 91

Table 16. Temperature dependences, stoichiometric parameters, composition parameters and parameters describing oxygen transfer in the CWM1 biokinetic model [*Langergraber et al.,* 2009]. 93

Table 17. Definition of terms related to geometry design. 96

Table 18. Definition of terms related to boundary discretization. 165

Table 19. Finite element mesh sections generated in different HYDRUS versions. 169

Table 20. Definition of commands used to manipulate Property Objects. 185

Table 21. Standard variables displayed in the View Window of the Results tab (Results - Graphical Display). 194

Table 22. Alternative variables that can be displayed in the View Window of the Results tab. 195

Table 23. Definition of various concentration modes (for linear sorption model). 196
Table 24. Graph options in the HYDRUS interface. 207
Table 25. HYDRUS menu commands. 232
Table 26. Brief description of HYDRUS menu commands.....239

Abstract

Šejna, M., J. Šimůnek, and M. Th. van Genuchten, The HYDRUS Software Package for Simulating Two- and Three-Dimensional Movement of Water, Heat, and Multiple Solutes in Variably-Saturated Media, User Manual, Version 2.0, PC Progress, Prague, Czech Republic, 280 pp., 2011.

This report documents version 2.0 of the **Graphical User Interface of HYDRUS**, a software package for simulating water, heat, and solute movement in two- and three- dimensional variably saturated media. The software package consists of the computational computer program, and the interactive graphics-based user interface. The HYDRUS program numerically solves the Richards equation for variably saturated water flow and advection-dispersion equations for both heat and solute transport. The flow equation incorporates a sink term to account for water uptake by plant roots. The heat transport equation considers transport due to conduction and convection with flowing water. The solute transport equations consider advective-dispersive transport in the liquid phase, as well as diffusion in the gaseous phase. The transport equations also include provisions for nonlinear nonequilibrium reactions between the solid and liquid phases, linear equilibrium reactions between the liquid and gaseous phases, zero-order production, and two first-order degradation reactions. In addition, physical nonequilibrium solute transport can be accounted for by assuming a two-region, dual-porosity type formulation which partitions the liquid phase into mobile and immobile regions. Attachment/detachment theory, including filtration theory, is additionally included to enable simulations of the transport of viruses, colloids, and/or bacteria.

HYDRUS may be used to analyze water and solute movement in unsaturated, partially saturated, or fully saturated porous media. The program can handle flow regions delineated by irregular boundaries. The flow region itself may be composed of nonuniform soils having an arbitrary degree of local anisotropy. Flow and transport can occur in the two-dimensional vertical or horizontal plane, a three-dimensional region exhibiting radial symmetry about the vertical axis, or a fully three-dimensional domain. The two-dimensional part of this program also includes a Marquardt-Levenberg type parameter optimization algorithm for inverse estimation of soil hydraulic and/or solute transport and reaction parameters from measured transient or steady-state data for two dimensional problems. Details of the various processes and features included in HYDRUS are provided in the **Technical Manual** [*Šimůnek et al*., 2011].

The main program unit of the **HYDRUS Graphical User Interface** (GUI) defines the overall computational environment of the system. This main module controls execution of the program and determines which other optional modules are necessary for a particular application. The module contains a project manager and both the pre-processing and post-processing units. The pre-processing unit includes specification of all necessary parameters to successfully run the **HYDRUS** FORTRAN codes, grid generators for relatively simple rectangular and hexahedral transport domains, a grid generator for unstructured finite element meshes for complex two-dimensional domains, a small catalog of soil hydraulic properties, and a Rosetta Lite program for generating soil hydraulic properties from soil textural data. The post-processing unit consists of simple *x-y* graphics for graphical presentation of soil hydraulic properties, as well as such output as distributions versus time of a particular variable at selected observation points, and actual or cumulative water and

solute fluxes across boundaries of a particular type. The post-processing unit also includes options to present results of a particular simulation by means of contour maps, isolines, spectral maps, and velocity vectors, and/or by animation using both contour and spectral maps.

Version 2.0, which includes the 3D-Professional Level of HYDRUS, includes many new features as compared to version 1.0. New features and changes in the HYDRUS GUI:

1) Supports for complex general three-dimensional geometries (Professional Level).
2) Domain Properties, Initial Conditions, and Boundary Conditions can be specified on Geometrical Objects (defining the transport domain) rather than on the finite element mesh.
3) Import of initial conditions from existing HYDRUS projects even with (slightly) different geometry or FE mesh.
4) Import of various quantities (e.g., domain properties, initial and boundary conditions) from another HYDRUS projects even with (slightly) different geometry or FE mesh.
5) Support of ParSWMS (a parallelized version of SWMS_3D).
6) Support of UNSATCHEM (a module simulating transport of and reactions between major ions).
7) The Mass Balance (Inverse) Information dialog window enables to display texts larger than the capacity of the Edit window.
8) Root distribution can be specified using GUI parallel with the slope for hillslopes.
9) Display of results using Isosurfaces.
10) Support of a new CWM1 constructed wetland module [*Langergraber et al*., 2009].

New features and changes in the HYDRUS in the computational modules:

1) New initializations conditions for solute transport (initial conditions can be specified in the total solute mass and nonequilibrium phases can be initially equilibrated).
2) Various new boundary conditions (e.g., gradient, surface drip, subsurface drip, and seepage face with a specified pressure head boundary conditions).
3) Triggered Irrigation - irrigation is triggered by the program when the pressure head at a particular observation node drops below a specified value.
4) HYDRUS calculates and reports surface runoff, evaporation and infiltration fluxes for the atmospheric boundary.
5) Water content dependence of solute reactions parameters using the *Walker*'s [1974] formula was implemented.
6) A new option to consider root solute uptake, including both passive and active uptake [*Šimůnek and Hopmans*, 2009].
7) The Per Moldrup's tortuosity models [*Moldrup et al*., 1997, 2000] were implemented as an alternative to the *Millington and Quirk* [1960] model.
8) An option to use a set of Boundary Condition records multiple times.
9) Executable programs are about 1.5 - 3 times faster than in the standard version due to the loop vectorization.
10) Options related to the fumigant transport (e.g., removal of tarp, temperature dependent tarp properties, additional injection of fumigant).
11) A new CWM1 constructed wetland module [*Langergraber et al*., 2009].

This report serves as a **User Manual** and reference document of the **Graphical User Interface** of the **HYDRUS** software package. Technical aspects such as governing equations and details about the invoked numerical techniques are documented in a separate **Technical Manual**.

Introduction to the HYDRUS Graphical User Interface

The past several decades or so has seen an explosion of increasingly sophisticated numerical models for simulating water flow and contaminant transport in the subsurface, including models dealing with one- and multi-dimensional flow and transport processes in the unsaturated or vadose zone between the soil surface and the ground water table. Even with an abundance of well-documented models now available, one major problem often preventing their optimal use is the extensive work required for data preparation, numerical grid design, and graphical presentation of the output results. Hence, the more widespread use of multi-dimensional models requires ways which make it easier to create, manipulate and display large data files, and which facilitate interactive data management. Introducing such techniques will free users from cumbersome manual data processing, and should enhance the efficiency in which programs are being implemented for a particular example. To avoid or simplify the preparation and management of relatively complex input data files for two- and three-dimensional applications, and to graphically display the final simulation results, we developed an interactive graphics-based user-friendly interface HYDRUS for the MS Windows 95, 98, NT, ME, XP, Vista, and 7 environments. The interface is connected directly to the computational codes. The current version 2.0 of the HYDRUS graphical user interface represents a major upgrade of version 1.0, which itself was a complete rewrite of the version 2.0 of HYDRUS-2D that expanded capabilities of HYDRUS-2D to three-dimensional problems. Version 2, which includes the 3D-Professional Level of HYDRUS, includes many new features as compared to version 1.0. In particular, it includes support for complex general three-dimensional geometries and an option to specify various domain properties, and initial and boundary conditions on geometrical objects, rather than directly on the finite element mesh.

In addition to information given in this user manual, extensive context-sensitive on-line help is made part of the graphical user interface (GUI). By holding the F1 button or clicking on the Help button while working in any window, the user obtains information about the window content. In addition, context-sensitive help is available in every module using the "SHIFT+F1" help button. In this mode, the mouse cursor changes to a help cursor (a combination arrow + question mark), which a user can use to select a particular object for which help is needed (e.g., a menu item, toolbar button, or other features). At that point, a help file will be displayed giving information about the item on which the user clicked. Except for the computational modules that are written in FORTRAN, the entire GUI is written in C++.

The HYDRUS Graphical User Interface (Fig. 1) is the main program unit defining the overall computational environment of the system. This main module controls execution of the program and determines which other optional modules are necessary for a particular application. The module contains a project manager and both the pre-processing and post-processing units. The pre-processing unit includes specification of all necessary parameters to successfully run the **HYDRUS** FORTRAN codes (modules H2D_CALC, H2D_CLCI, H2D_WETL, H2D_UNSC, and/or H3D_CALC), grid generators for relatively simple rectangular and hexahedral transport domains, a grid generator for unstructured finite element meshes appropriate for more complex two-dimensional domains, a small catalog of soil hydraulic properties, and a Rosetta Lite program for generating soil hydraulic properties from textural information. The post-processing unit consists of simple *x-y* graphs for graphical presentation of the soil hydraulic properties, distributions versus time of a particular variable at selected observation points, as well as actual or cumulative water and

solute fluxes across boundaries of a particular type. The post-processing unit also includes options to present results of a simulation by means of contour maps, isolines, isosurfaces, spectral maps, and velocity vectors, and/or by animation using both contour and spectral maps.

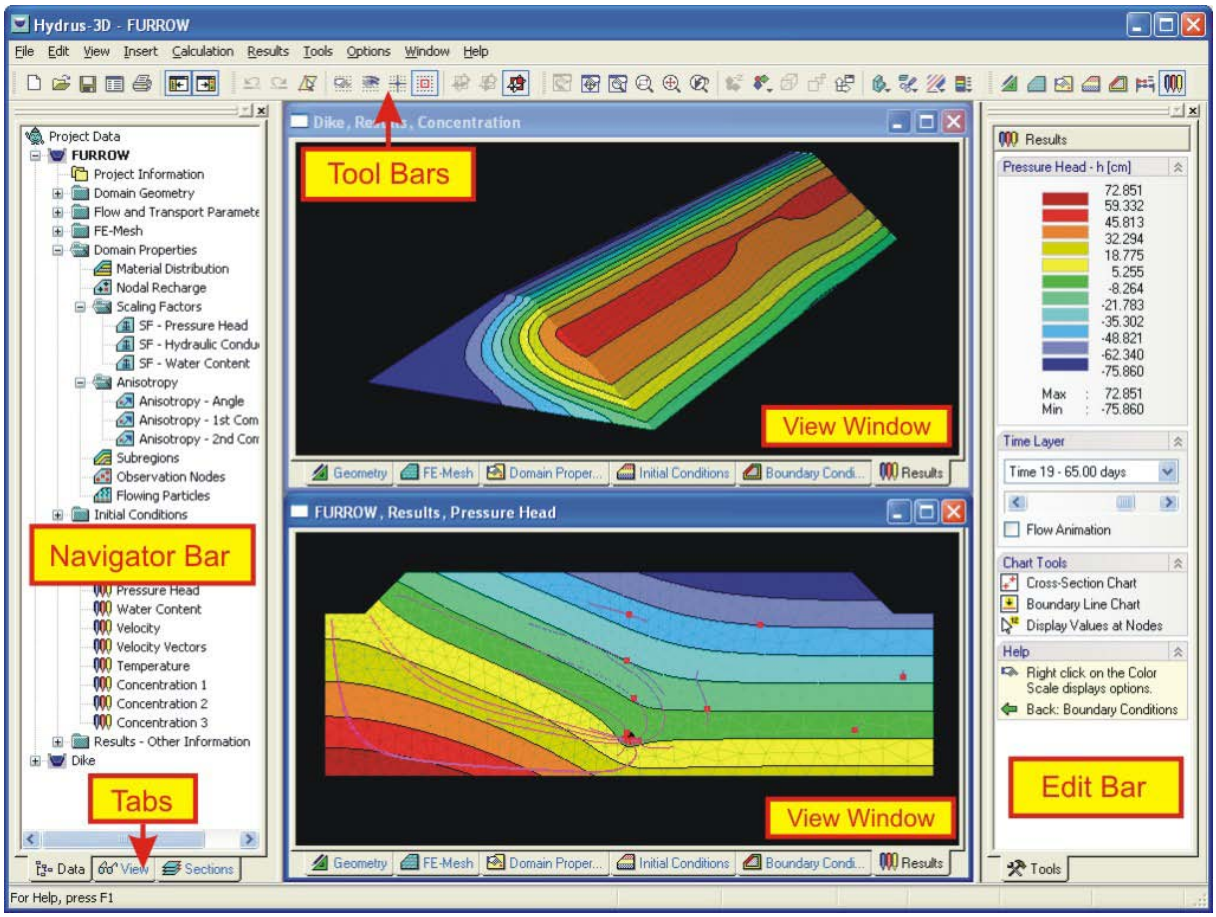


Figure 1. The HYDRUS Graphical User Interface (the main window).

Figure 1 shows the main window of the HYDRUS graphical user interface, including its main components such as the **Menu**, **Toolbars**, the **View Window**, the **Navigator Bar**, **Tabs**, and the **Edit Bar**. These terms will be used throughout this user manual. The text below provides a detailed description of all major components of the graphical user interface. At the end of this user manual a list is given of all commands accessible through the menu (Table 25), as well as a brief discussion of the action taken with particular commands (Table 26). More detailed descriptions are available through the on-line help.

Work for a new project should begin by opening the Project Manager (see Chapter 1), and giving a name and brief description to the new project. Next the **Domain Type and Units** dialog Window (Figs. 6 and 7) appears (this window can be also selected from the Pre-processing Menu). From this point on the program will navigate users through the entire process of entering input files. Users may either select particular commands from a menu, or allow the interface to lead them through the process of entering input data by selecting the Next button. Alternatively, clicking the Previous button will return users to the previous window. Pre- and post processing commands and processes

are also sequentially listed on the **Data Tab** of the **Navigator Bar**. Green arrows on the **Edit Bar** always direct users to subsequent or previous input processes for a particular command. Many commands and processes can be alternatively accessed using either the **Toolbars** and **Menus**, or the **Navigator** and **Edit Bars**.

1. Project Manager and Data Management

A **Project Manager** (called by the command *File->Project Manager*, Figs. 2 and 3) is used to manage the data of existing projects, and helps to locate, open, copy, delete and/or rename desired projects or their input or output data. A **Project** represents any particular problem to be solved by HYDRUS. The project name, as well as a brief description of the project (Fig. 4), helps to locate a particular problem. Projects are represented by a file *project_name.h3d2* (the final 2 refers to version 2 of HYDRUS; extension h3d was used with version 1.0) that contains all input and output data when the *Temporary Working Directory* option (Fig. 4) is used. It contains only the input data when the *Permanent Working Directory* option is selected. HYDRUS input files (used by the computational modules) are extracted from the *project_name.h3d2* file into a working subdirectory; output data created by the calculation module are sent into the same folder. When saving a project, output files (created by the computational modules) are also included into the *project_name.h3d2* file (when the *Temporary Working Directory* option is used). The input and output files can be either permanently kept in the external working directory, or are stored in this folder only during calculations (Fig. 4, the radio buttons *Temporary – is deleted after closing the project* and *Permanent – result files are kept in this directory*). The location of the external working directory is specified in the **Project Description** (Fig. 4) and the **Program Options** dialog window (Fig. 150).

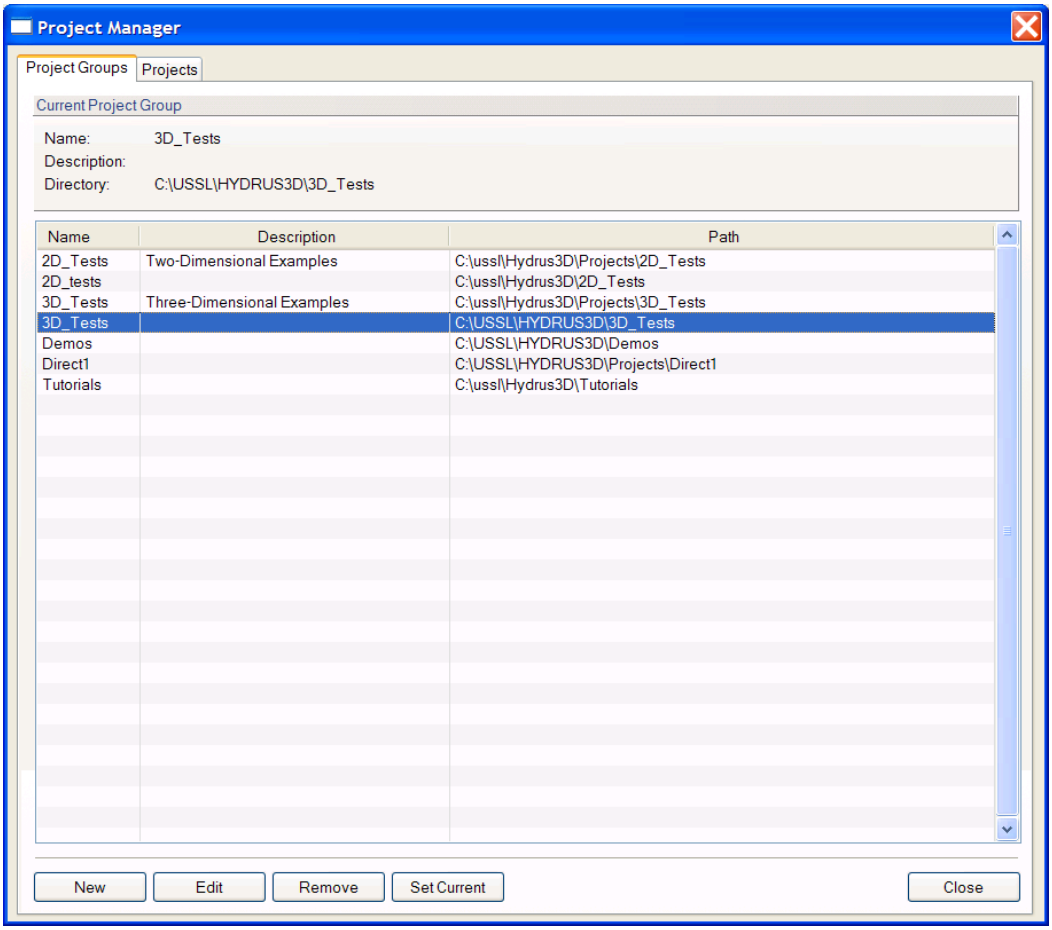


Figure 2. The project Manager with the Project Groups tab.

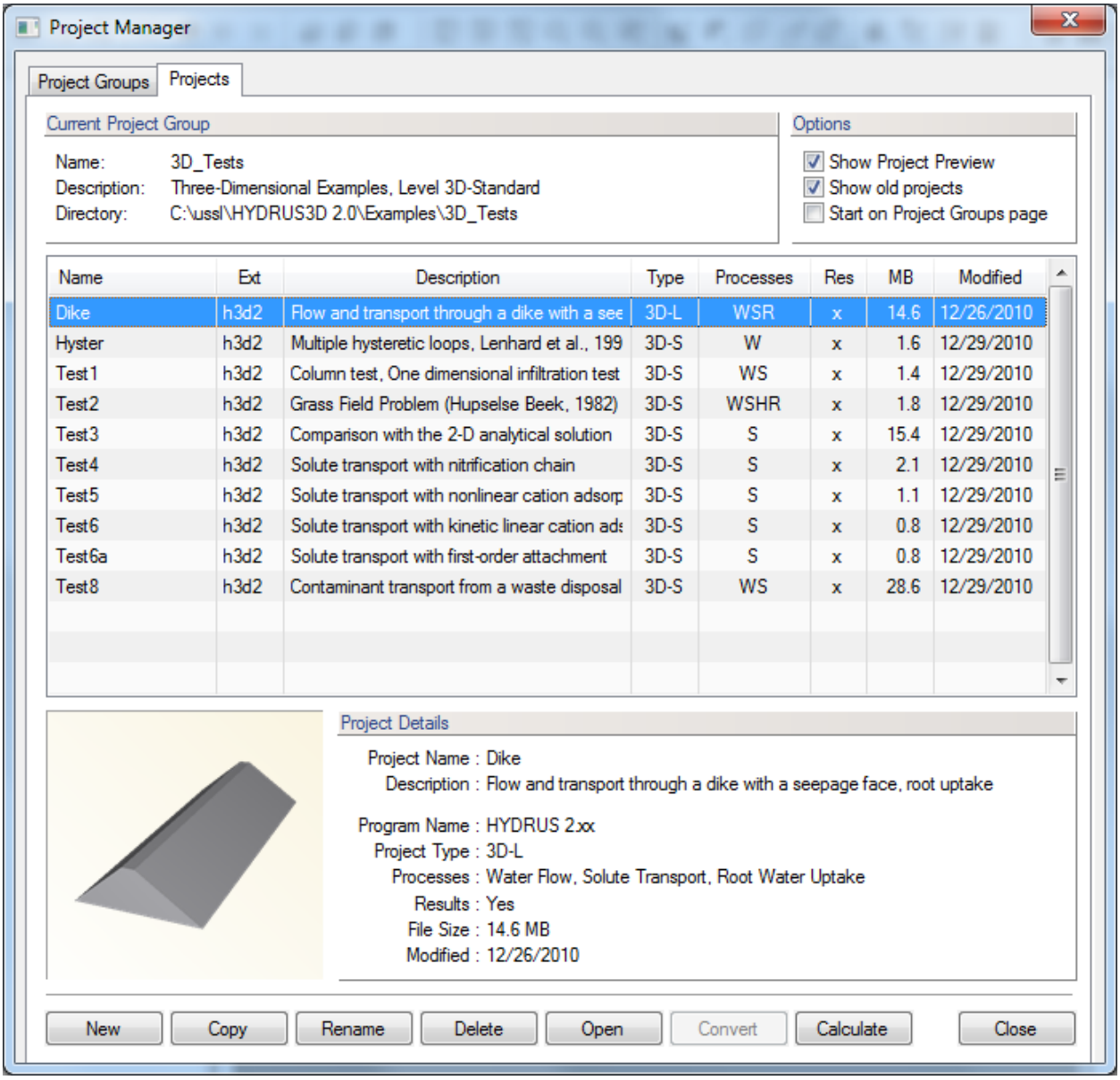

Project Manager
Project Groups
Projects
Current Project Group
Name: 3D_Tests
Description: Three-Dimensional Examples, Level 3D-Standard
Directory: C:\ussl\HYDRUS3D 2.0\Examples\3D_Tests
Options
Show Project Preview
Show old projects
Start on Project Groups page
Name Ext Description Type Processes Res MB Modified
Dike h3d2 Flow and transport through a dike with a see 3D-L WSR x 14.6 12/26/2010
Hyster h3d2 Multiple hysteretic loops, Lenhard et al., 199 3D-S W x 1.6 12/29/2010
Test1 h3d2 Column test, One dimensional infiltration test 3D-S WS x 1.4 12/29/2010
Test2 h3d2 Grass Field Problem (Hupselse Beek, 1982) 3D-S WSHR x 1.8 12/29/2010
Test3 h3d2 Comparison with the 2-D analytical solution 3D-S S x 15.4 12/29/2010
Test4 h3d2 Solute transport with nitrification chain 3D-S S x 2.1 12/29/2010
Test5 h3d2 Solute transport with nonlinear cation adsorp 3D-S S x 1.1 12/29/2010
Test6 h3d2 Solute transport with kinetic linear cation ads 3D-S S x 0.8 12/29/2010
Test6a h3d2 Solute transport with first-order attachment 3D-S S x 0.8 12/29/2010
Test8 h3d2 Contaminant transport from a waste disposal 3D-S WS x 28.6 12/29/2010
Project Details
Project Name : Dike
Description : Flow and transport through a dike with a seepage face, root uptake
Program Name : HYDRUS 2.xx
Project Type : 3D-L
Processes : Water Flow, Solute Transport, Root Water Uptake
Results : Yes
File Size : 14.6 MB
Modified : 12/26/2010
New
Copy
Rename
Delete
Open
Convert
Calculate
Close

Figure 3. The Project Manager with the Projects tab.

The **Project Manager** gives users considerable freedom in organizing their projects. The projects are grouped into **Project Groups** (Fig. 2), which can be placed anywhere in accessible memory (i.e., on local and/or network hard drives). **Project Groups** serve to organize projects into logical groups defined by a user. Each **Project Group** has its own *name*, *description*, and *pathway* (Figs. 2 and 5). A **Project Group** can be any existing accessible subdirectory (folder). HYDRUS is installed together with two default Project Groups, *2D_Tests* and *3D_Tests*, which are located in the HYDRUS3D folder. The *2D_Tests* and *3D_Tests* Project Groups contain test examples for two- and three-dimensional problems, respectively. We suggest that users create their own Project Groups (e.g., the *My_2D_Direct*, *My_2D_Inverse*, and *My_3D_Direct* Project Groups), and keep the provided examples intact for future reference. Projects can be copied with the **Project Manager** only within a particular Project Group. Users can copy projects between Project Groups (or share

their HYDRUS projects with colleagues and clients) using standard file managing software, such as Windows Explorer. In that case one must copy only the *project_name.h3d2* file (when the radio buttons *Temporary – is deleted after closing the project* is used, Fig. 4). When temporary data are kept permanently in the working directory (i.e., the radio button *Permanent – results files are kept in this directory* is selected, Fig. 4), the working directory must be copied together with the *project_name.h3d2* file.

In addition to a *Name* and a brief *Description* of a **Project**, the **Project Manager** also displays dimensions for a particular problem (*Type*: the dimensions are either 2D or 3D, and the geometry is either Simple (S), Layered (L), or General (G), see Section 2), what *Processes* are involved (W – water flow, S – solute transport, T – heat transport, R – root water uptake, Inv – Inverse problem), the size of the project (MB), when the project was created (*Date*) and whether or not the *Results* exist (Fig. 3). The **Project Manager** can also display a preview of the **Project**'s geometry (see the check box *Show Project Preview* in Fig. 3). Commands of the **Project Manager** are listed in Table 1.

Table 1. Commands in the **Project Manager**.

Group	Command	Description
Project Group	New	Registers a new Project Group in the Project Manager.
	Edit	Renames the selected Project Group, and changes its description and/or location.
	Remove	Removes registration of a selected Project Group from the Project Manager.
	Set As Current	Sets a selected Project Group as the active Project Group.
	Close	Closes the Project Manager.
Project	New	Creates a new project in the current Project Group.
	Copy	Copies a selected project within the current Project Group.
	Rename	Renames a selected project.
	Delete	Deletes a selected project.
	Open	Opens a selected project.
	Close	Closes the Project Manager.
	Convert	Converts projects created by earlier HYDRUS versions (i.e., either HYDRUS-2D or version 1.0 of HYDRUS (2D/3D)).
	Calculate	Calculates selected HYDRUS projects. This command allows users to calculate multiple selected projects simultaneously.

Options	Description
Show Project Preview	Provides a preview of the geometry of a particular project in the bottom left corner of the Project Manager.
Show Old Projects	Shows projects created using earlier HYDRUS versions, i.e., either HYDRUS-2D or version 1.0 of HYDRUS (2D/3D).
Start on Project Groups Page	Opens the Project Manager at the Project Groups Tab.

The commands **New** and **Rename** from the **Project Tab** of the **Project Manager** dialog window (Fig. 3) call the **Project Information** dialog window (Fig. 4), which contains the *Name* and *Description* of the project, as well as information about the **Project Group** (name, description, and pathway) to which the project belongs. It also contains information whether or not the input and output data are kept permanently in an external directory (the radio buttons *Temporary – is deleted after closing the project* and *Permanent – result files are kept in this directory*, Fig. 4).

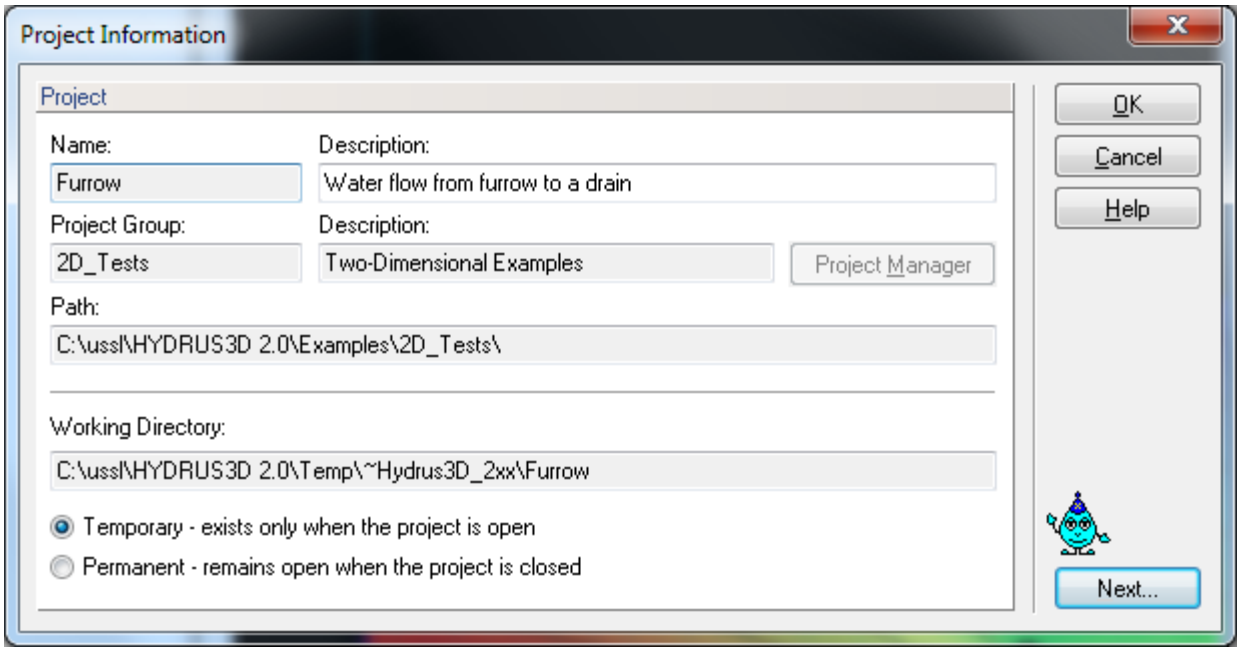


Figure 4. The Project Information dialog window.

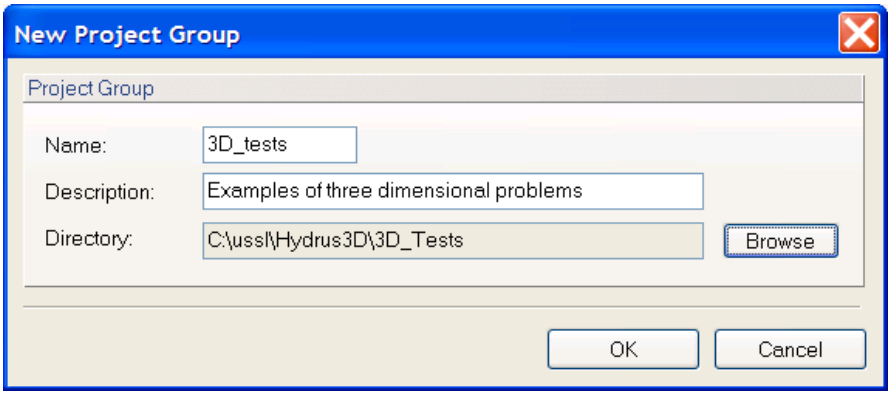


Figure 5. General description of the HYDRUS Project Group.

Projects created by the previous versions of HYDRUS (e.g., HYDRUS-2D) can be imported into the current version of HYDRUS using two ways:

A. Individual projects can be converted using the command *File->Import and Export->Import HYDRUS-2D Project*. This is done by first creating a new **Project**, and then selecting the above command and browsing for the location of a project created with a previous version of HYDRUS-2D. The input data of the older project are then converted into the new HYDRUS format. Results of the older project can then be viewed using the new version of HYDRUS, while projects can be modified or recalculated as needed.

B. Multiple HYDRUS-2D projects (or HYDRUS projects created by earlier versions of HYDRUS) can be converted simultaneously using the **Convert** command of the **Project Manager**. One first creates a HYDRUS Project Group for a folder in which the HYDRUS-2D projects are located and selects the **Show Old Projects** option at the **Project Tab** of the **Project Manager**. One then selects projects to be converted and clicks the **Convert** command. HYDRUS in this way creates HYDRUS projects and stores all input and output files in the **project_name.h3d2** files.

Input data can be edited either using the HYDRUS graphical user interface (this modifies directly the *project_name.h3d2* file) or the input data can be modified manually. In such case, HYDRUS input files need to be stored in the working external directory (sent there by the command *File->Import and Export->Export Data for HYDRUS Solver*), and then can be imported back into the HYDRUS *project_name.h3d2* file using the command *File->Import and Export->Import Input Data from *.In Files*.

The **Working Directory** is a folder into which the program stores temporary data. Each open project has its own Working Directory, where the program stores, for example, input files for computational modules, and where computational modules write the output files. When saving a project, data from the Working Directory are copied into the main project file *project_name.h3d2*. When the project is closed, the Working Directory is deleted. Only when a user selects the option "*Permanent – result files are kept in this directory*" (Fig. 4) is the Working Directory not deleted after closing the project, in which case the temporary data are not copied into the main project file.

2. Projects Geometry Information

In the first dialog window that a user encounters after creating a new project, he/she needs to specify whether the flow and transport problem occurs in two- or three-dimensional transport domains. Geometry type is selected in the **Domain Type and Units** dialog Window (Fig. 6 and 7). In this dialog window, users specify the **Type of Geometry**, the **2D Domain Options**, the **Length Units**, and the size of the **Initial Project Group** (the approximate size of the transport domain).

Type of Geometry: This section allows a user to choose between simple geometries having a structured finite element mesh (i.e., **2D-Simple (Parametric)** and **3D-Simple (Parametric)**), or more general geometries having an unstructured finite element mesh (i.e., **2D-General (Boundary Rep.)**, **3D-Layered**, and **3D-General (Boundary Rep.)**). Available options depend on the level of authorization (purchased License). Only simple geometries **2D-Simple (Parametric)** and **3D-Simple (Parametric)** are available for HYDRUS Levels **2D-Lite** and **3D-Lite**, respectively. **2D-General (Boundary Rep.)** is available for the **2D-Standard** Level, **3D-Layered** for the **3D-Standard** Level, and **3D-General (Boundary Rep.)** for the **3D-Professional** Level.

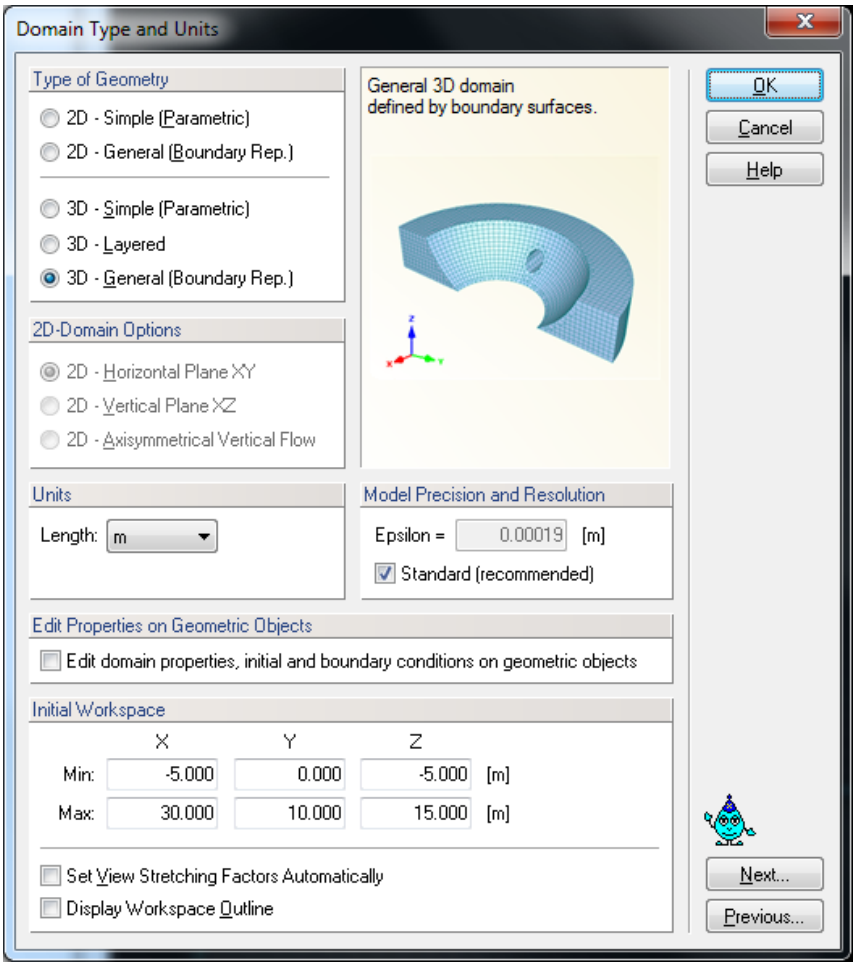


Figure 6. The Domain Type and Units dialog window (with 3D preview).

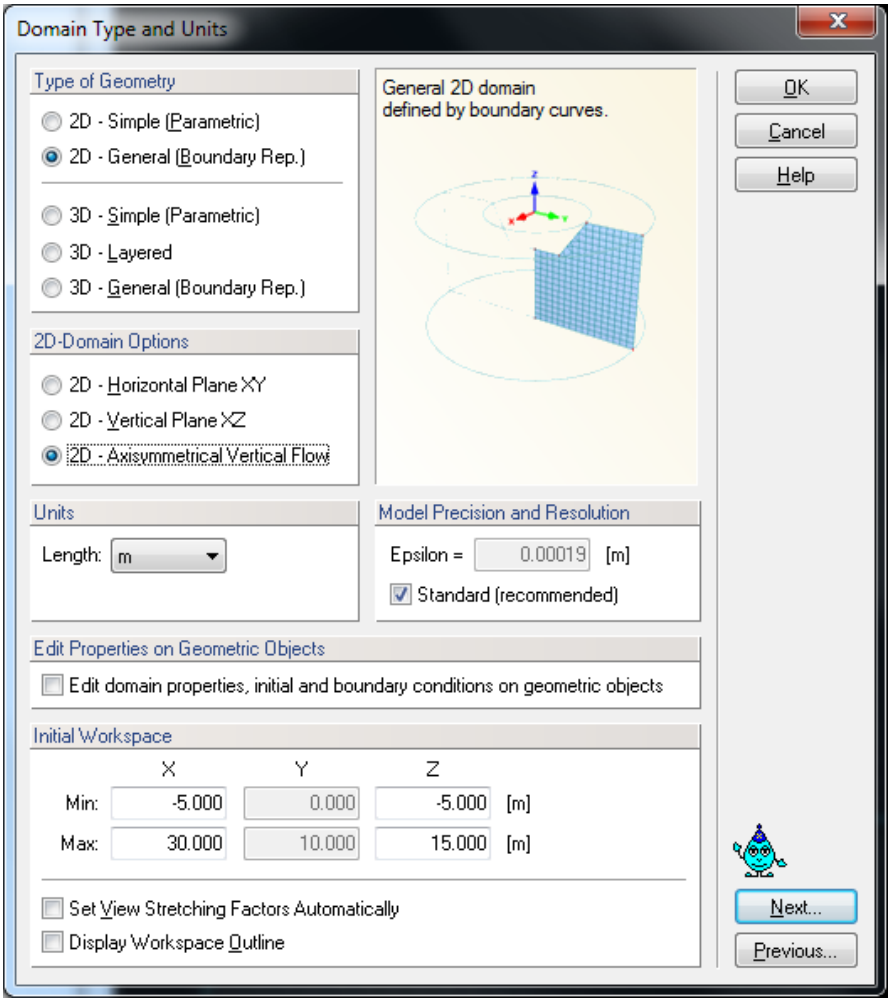


Figure 7. The Domain Type and Units dialog window (with 2D axisymmetrical preview).

There are two types of two-dimensional transport domains (Surfaces, see also Section 4.2) depending upon the selection made in the Domain Type and Units dialog window (Fig. 6 and 7):

- **2D-Simple (Parametric):** This type of solid has a **Rectangular Shape** and is defined by its basic dimensions. Rectangular domains are defined by three straight lines, one at the bottom of the domain and two at the sides, whereas the upper boundary may or may not be straight. Nodes along the upper boundary line may in that case have variable *x*- and *z*-coordinates. However, the lower boundary line must always be horizontal (or have a specified slope), while the left and right boundary lines must be vertical. The flow region is then discretized into a structured triangular mesh. Examples of simple rectangular geometries are shown in Figure 8 (top).
- **2D-General (Boundary Rep.):** This type of Surface is defined by a set of **Boundary Curves** see Section 4.2). Examples of general two-dimensional geometries are shown in Figure 8 (bottom) and Figure 42.

There are three types of three-dimensional transport domains (Solids, see also Section 4.4) depending upon the selection made in the Domain Type and Units dialog window (Fig. 6 and 7):

- **3D-Simple (Parametric):** This type of solid has a **Hexahedral Shape** and is defined by its basic dimensions. The base can have a certain slope in the X and Y dimensions (Fig. 9). Hexahedral domains must have similar properties as rectangular domains, i.e., vertical planes at the sides, a horizontal (or with a specified slope) plane at the bottom boundary, and with only the upper boundary not needing to be a plane. An example of a simple hexahedral three-dimensional geometry (i.e., 3D-Simple) is given in Figure 9.
- **3D-Layered:** This type of solid is defined by the **Base Surface** (see Section 4.2) and one or more **Thickness Vectors** (see Section 4.5).
- **3D-General (Boundary Rep.):** This type of solid is defined using a set of surfaces that fully form its boundaries. This type of geometries is available only in the **3D-Professional** version. **3D-General Geometries** can be formed from three-dimensional objects (**Solids**) of general shapes. Three-dimensional objects are formed by boundary surfaces, which can be either **Planar** surfaces or **Curved** surfaces (**Quadrangle**, **Rotary**, **Pipe**, or **B-Spline**).

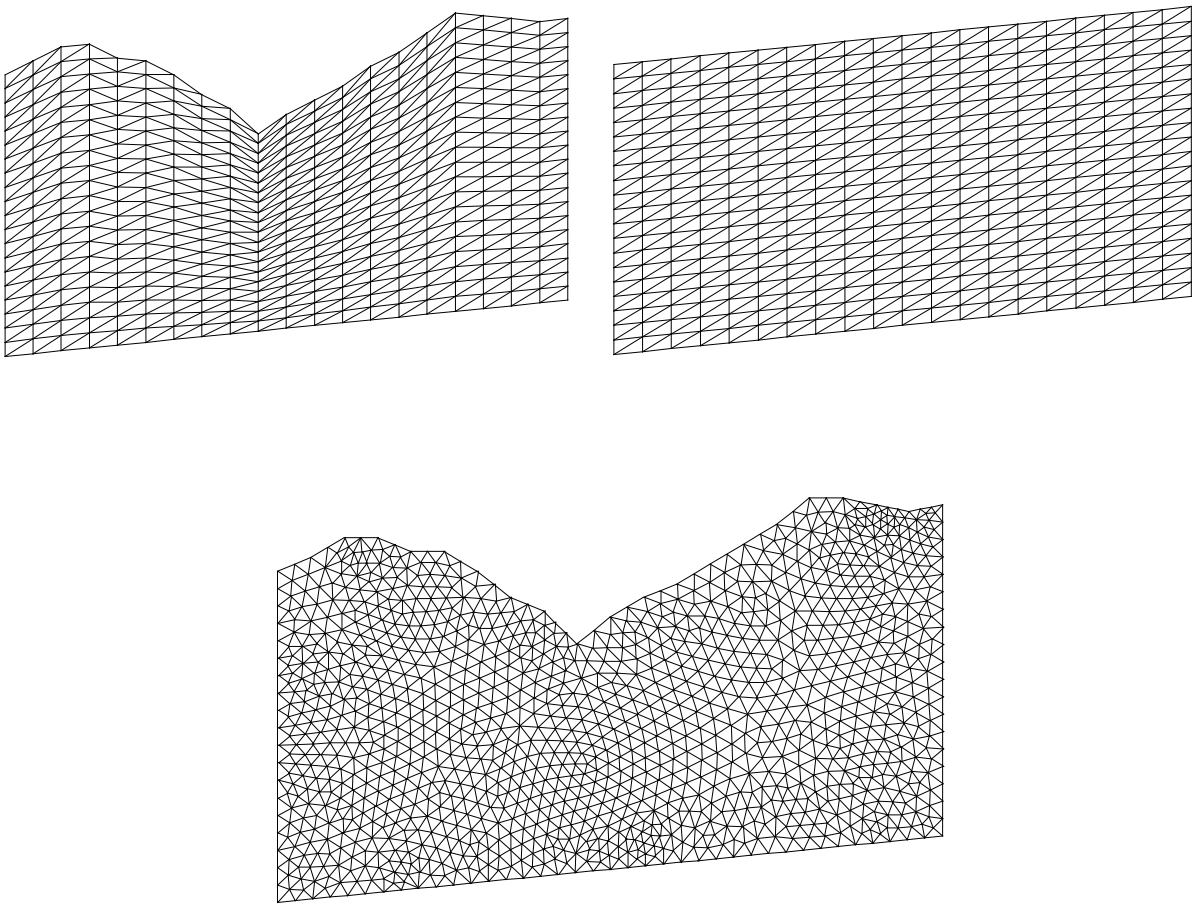


Figure 8. Examples of rectangular (top) and general (bottom) two-dimensional geometries.

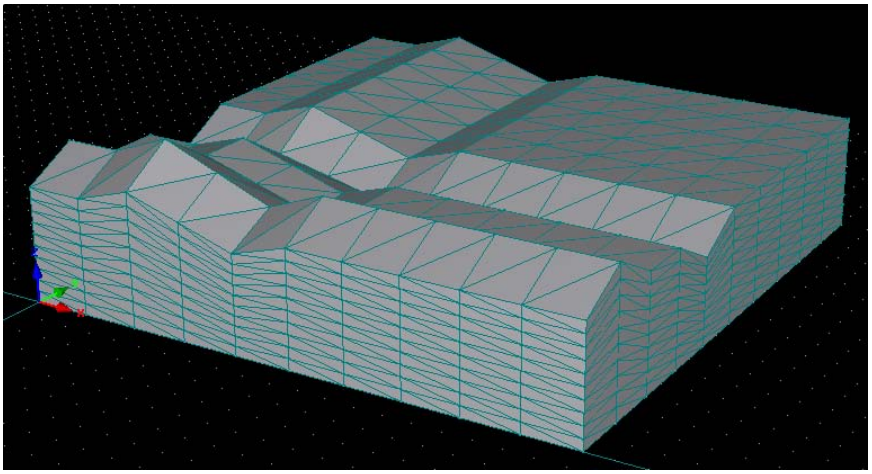


Figure 9. Example of a hexahedral three-dimensional geometry.

2D-Domain Options: Two-dimensional flow and transport can occur in a horizontal or vertical plane, or in an axisymmetrical quasi-three-dimensional transport domain. When a three-dimensional axisymmetrical system is selected, the *z*-coordinate must coincide with the vertical axis of symmetry. A typical example of the selected 2D or 3D geometry is shown in the preview part of the dialog window.

The simple geometries are defined in the *Rectangular* (Fig. 10) or *Hexahedral Domain Definition* (Fig. 11) dialog windows for two-dimensional and three-dimensional problems, respectively. In each of these windows, users need to specify the vertical and horizontal dimensions of the transport domain, as well as a possible slope of the base of the domain in different directions (if applicable; α is in the *x*-direction and β is in the *y*-direction). The preview in the middle of the dialog window of a simple example showing all geometry parameters should help users in specifying their desired transport domain (*Dimensions* and *Slope*).

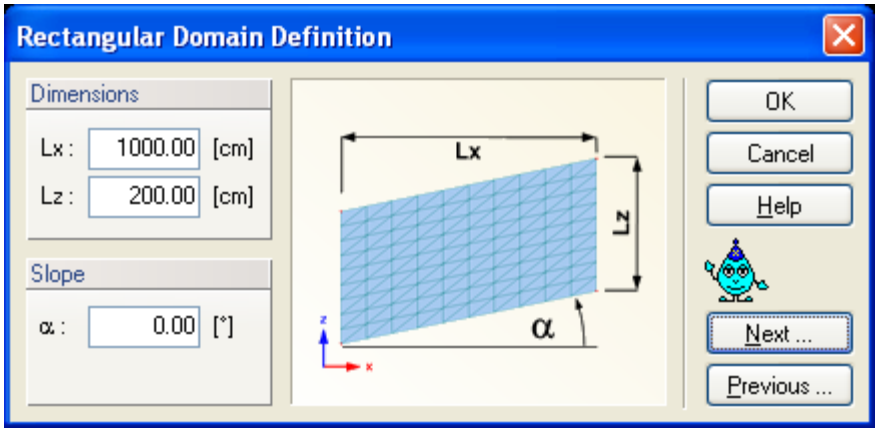


Figure 10. The Rectangular Domain Definition dialog window.

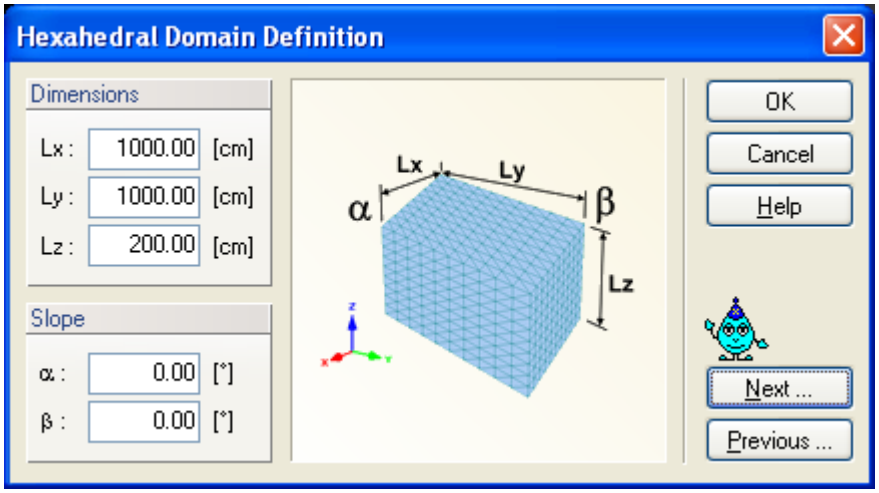


Figure 11. The Hexahedral Domain Definition dialog window.

In the **Domain Type and Units** dialog Window (Figs. 6 and 7) users also select the geometry **Units** to be used throughout the application (mm, cm, m) and the size of the **Initial Project Group**. When units are changed during specification or after reading the input data, then all input variables are automatically converted into the new units.

Initial Project Group: This part of the dialog allows users to define the initial dimensions of the graphical view window.

Model Precision and Resolution: *Epsilon* is a minimum resolution recognized when defining geometrical objects. *Epsilon* is by default defined as *R*/100,000, where *R* is a domain radius, i.e., a radius of a circle/sphere circumscribing the domain. *Epsilon* is used, for example, for evaluation of positions of two points. If their distance is less than *Epsilon*, then the two points are replaced by a single point. A user-defined epsilon may lead to unstable behavior of the program and it is intended only for advanced users who may need it for special purposes. A correct functionality of geometrical calculations and generation of FE-meshes is not guaranteed for user-defined epsilons.

Edit Properties on Geometric Objects: When the check box "Edit domain properties, initial and boundary conditions on geometric objects" is checked, users can specify various properties and conditions on the Geometric Objects (See Section 6.5 "Defining Properties on Geometrical Objects" for details), rather than only on FE-Mesh, as available in Version 1.0 of HYDRUS. This option will be by default "On" for new projects, and it is "Off" for projects converted from Version 1.0. Users can turn this option "Off" and continue defining various properties on FE-Mesh, as they have been used to. Users can turn this option "On" for projects converted from Version 1.0 of HYDRUS. However, they will then lose their original definitions and will have to specify them again on Geometric Objects.

3. Flow Parameters

3.1. *Main Processes*

In the **Main Processes** dialog window (Fig. 12), users specify the processes to be simulated, i.e., water flow, multiple solute transport, heat transport, and/or root water uptake. The major ion chemistry module [UNSATCHEM; *Šimůnek and Suarez*, 1994] can be used instead of the standard solute transport module. Since there is currently no technical manual describing the two-dimensional version of the UNSATCHEM module, users are referred to the HYDRUS-1D manual [*Šimůnek et al.,* 2008], which provides all relevant information about this module.

The program automatically considers transient water flow when the "water flow" option is selected. Otherwise the code tries to calculate steady-state flow from the specified initial and boundary conditions. The success of such calculations depends on the complexity and/or nonlinearity of the problem. If unsuccessful, then a model run with constant boundary conditions and long simulation time may be required.

If the solute transport, heat transport or root water uptake options originally considered in an existing project are switched off by the user, the program issues a warning that all data related to these processes will be lost. If this loss is undesirable we recommend that users first copy the input data of the current project to a new project before switching off the solute transport, heat transport and/or root water uptake options.

For two-dimensional problems a user can also select if a **Direct** or **Inverse problem** is to be solved. Inverse problems involve the estimation of selected parameters from available experimental data.

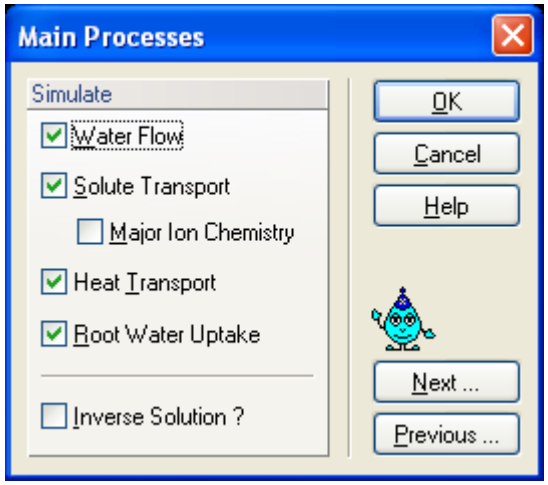


Figure 12. The Main Processes dialog window.

3.2. *Inverse Solution*

HYDRUS implement a Marquardt-Levenberg type parameter estimation technique (Šimůnek and Hopmans, 2002) for inverse estimation of soil hydraulic (Hopmans et al., 2002) and/or solute transport and reaction (Šimůnek et al., 2002) parameters from measured transient or steady-state flow and/or transport data. The **Inverse Solution** dialog window (Fig. 13) appears only when the **Inverse Problem** in the **Main processes** dialog window (Fig. 12) is selected. Users select which parameters (the soil hydraulic, solute transport and reaction, and/or heat transport parameters) are to be optimized (**Estimate …**) from the specified experimental data.

One also selects the method of **Weighting of Inversion Data** in the objective function. Users can choose between no weighting, weighting by mean ratios, or weighting by standard deviations. When no weighting is selected, one needs to supply weights for particular data points in the **Data for Inverse Solution** dialog window (Fig. 14). When weighting by mean ratio or weighting by standard deviation is selected, then the code calculates either the means or the standard deviations of the different data sets (e.g., water contents, pressure heads, concentrations, …) and adjusts the weights proportionally. These internal weights can still be multiplied by weights from the **Data for Inverse Solution** dialog window (Fig. 14).

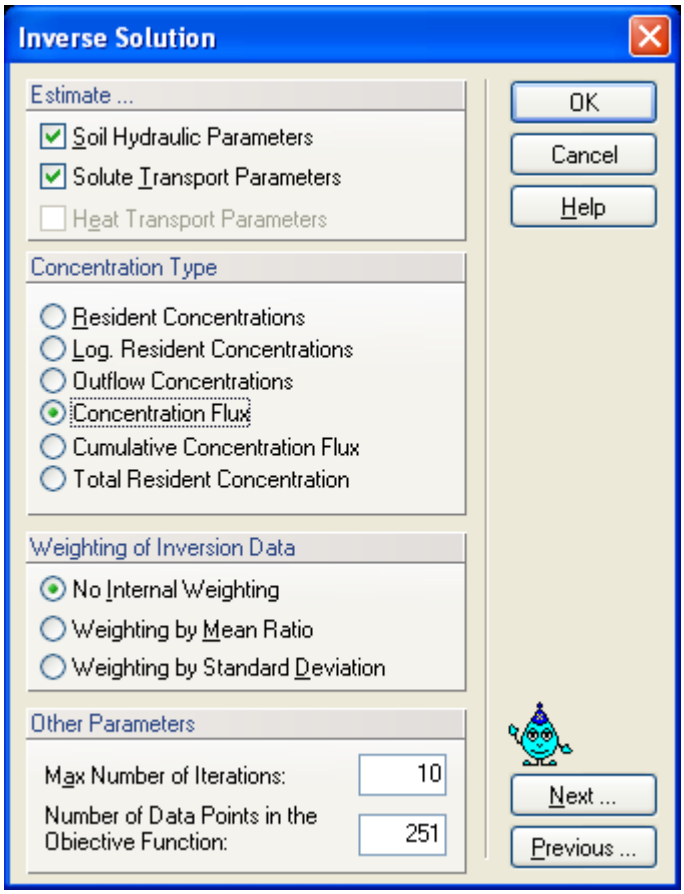
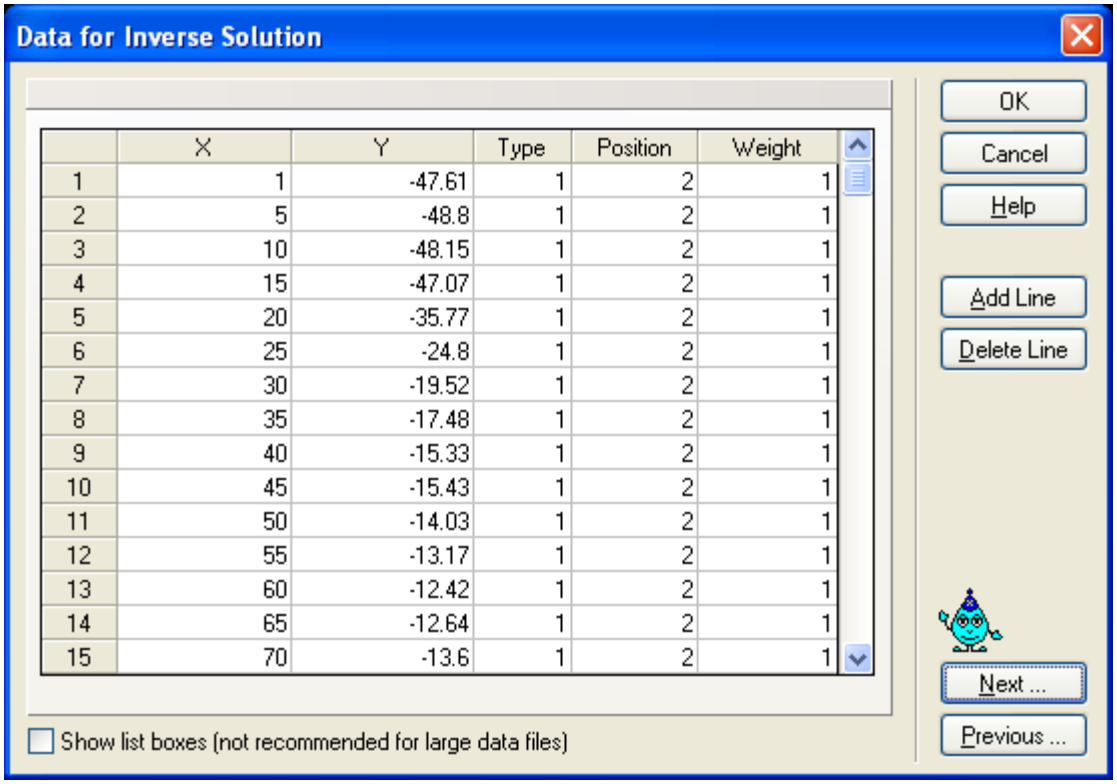


Figure 13. The Inverse Solution dialog window.

The objective function for the inverse estimation of solute transport parameter can be defined using different types of concentrations. Available **Concentration Types** are: a) the resident concentration in the liquid phase, b) a log-transformation of the resident concentration in the liquid phase, c) the outflow (flux) concentration, d) the solute concentration flux, e) the cumulative concentration (solute) flux, and f) the total resident concentration. The total resident concentration includes concentrations in the sorbed and nonequilibrium phases.

The maximum number of iterations for the inverse solution is also specified in this dialog window. If one selects zero number of iterations then only the direct simulation is carried out. However, users can still enter measured data, in which case the code compares results of the direct simulation with the measured data.



	X	Y	Type	Position	Weight
1	1	-47.61	1	2	1
2	5	-48.8	1	2	1
3	10	-48.15	1	2	1
4	15	-47.07	1	2	1
5	20	-35.77	1	2	1
6	25	-24.8	1	2	1
7	30	-19.52	1	2	1
8	35	-17.48	1	2	1
9	40	-15.33	1	2	1
10	45	-15.43	1	2	1
11	50	-14.03	1	2	1
12	55	-13.17	1	2	1
13	60	-12.42	1	2	1
14	65	-12.64	1	2	1
15	70	-13.6	1	2	1

Figure 14. The Data for Inverse Solution dialog window.

In the table Data for Inverse Solution (Fig. 14) one specifies the measured data that will be analyzed during the parameter optimization process. Many different types of data can be used to define the objective function that will be minimized for this purpose. How the values in the X and Y columns are interpreted depends on the Type and Position values. Weight is the weight associated with a particular data point. The following information can be included into the objective function:

Table 2. Data Types for the objective function (Inverse Problem).

Type	Data Point
0	Cumulative boundary fluxes across a specified boundary
1	Pressure head measurements at selected observation point(s)
2	Water content measurements at selected observation point(s)
3	Boundary flux across a specified boundary
4	Concentration or temperature measurements at observation point(s)
5	$h(\theta)$ measurements; soil water retention data
6	$K(h)$ measurements; hydraulic conductivity data point
7	Prior knowledge of parameter α
8	Prior knowledge of parameter n
9	Prior knowledge of parameter θ_r
10	Prior knowledge of parameter θ_s
11	Prior knowledge of parameter K_s

Depending upon the value of parameter **Type**, the first column (X) contains the following information:

Table 3. Definition of the column *X* in Fig. 14 based on Data Type (Inverse Problem).

X	Type
Time	0, 1, 2, 3, 4
Pressure head	5, 6
Dummy variable	7, 8, 9, 10, 11

Depending upon the value of parameter **Type**, the second (Y) and fourth (Position) columns contain the following information:

Table 4. Definition of the column *Y* in Fig. 14 based on Data Type (Inverse Problem).

Y	Type	Position
Cumulative boundary flux across a specified boundary	0	Code for the specified boundary*
Pressure head	1	Observation node number
Water content	2	Observation node number
Averaged water content of the entire flow domain	2	0
Averaged water content of the subregion	2	Negative subregion number
Concentrations/temperatures	4	Observation node number
Concentrations for the second solute	4	Negative observation node number
Total amount of solute in the entire flow domain	4	0
Boundary flux across a specified boundary	3	Code for the specified boundary*
Water content	5	Material number
Hydraulic conductivity	6	Material number
Particular parameter	7-11	Material number

*1 – constant pressure head or flux boundary; 2 – seepage face; 3 – variable pressure head or flux boundary 1; 4 – atmospheric boundary; 5 – drains; 6 – free or deep drainage boundary; 7, 8, and 9 – variable pressure head or flux boundaries 2, 3, or 4, respectively.

3.3. *Time Information*

The **Time Information** dialog window (Fig. 15) contains information associated with the **Time Discretization**, the **Time Units**, and the implementation of **Boundary Conditions**.

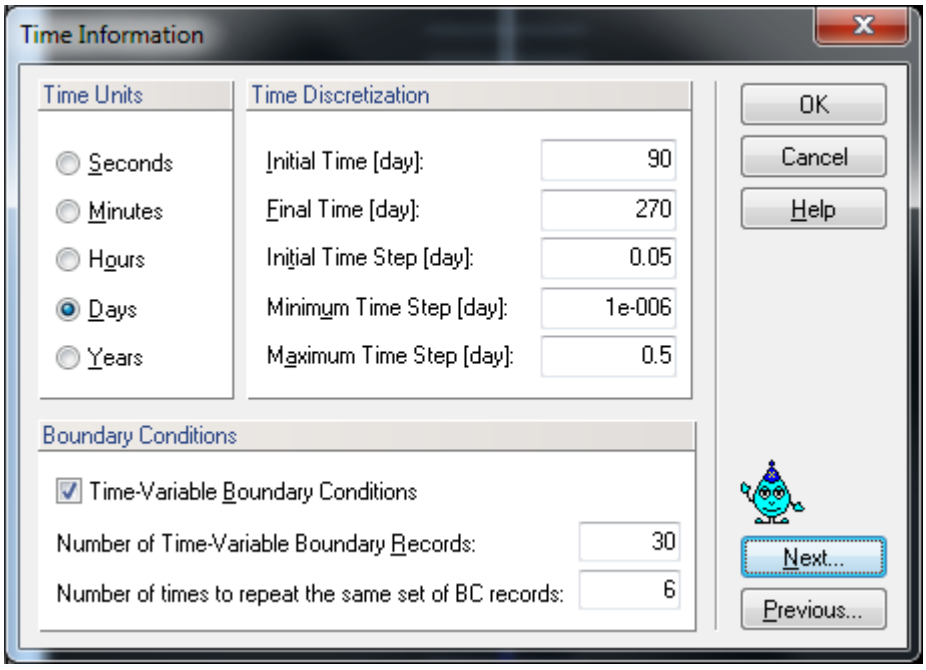


Figure 15. The Time Information dialog window.

Boundary Conditions

Time-Variable Boundary Condition - The **Number of Time-Variable Boundary Records** and time-dependent boundary conditions must be specified when this box is checked. The boundary conditions otherwise are assumed to be constant in time.

The same set of boundary records can be repeated number of times (**Number of times to repeat the same set of BC records**) (periodically) with a time period *tPeriod=tAtmLast-tInit*, where *tInit* is the **Initial Time** and *tAtmLast* is the time of the last specified time record. Note that *tMax< tInit +n*tPeriod*.

Table 5. Time Information variables.

Time Units	Time units [T] to be used throughout the application (years, days, hours, min, sec). When units are changed during or after data entry, then all input variables are converted automatically into the new units.
Initial Time	Starting time [T] of the calculation.
Final Time	Final time [T] of the calculation.
Initial Time Step	Initial time increment, Δt [T]. The recommended value for the initial time step depends on the type of simulation and boundary conditions used. When simulating a process that starts with a large initial pressure head or concentration gradient at the boundary (e.g., ponded infiltration or a sudden change of boundary concentration), use a small value of the initial time step (e.g., 1 s). When simulating a long term process with variable boundary conditions (e.g., seasonal or multiyear simulation), start with a larger time step (e.g., 15 min). This is because this initial time step is used whenever time variable boundary conditions significantly change (e.g., the water flux changes by 25% or more). If needed (if there is no convergence for Δt_{init}), the program will still use a smaller time step than Δt_{init}, but starting with larger Δt_{init} leads to more efficient calculations. In general smaller initial time steps must be used for soil with more nonlinear soil hydraulic properties (e.g., course textured soils) and larger initial time steps can be used for soil with less nonlinear soil hydraulic properties (e.g., loam).
Minimum Time Step	Minimum permitted value of the time increment, $\Delta t_{\min}$ [T]. The minimum time step must be smaller than a) the initial time step, b) interval between print times, and c) interval between time-variable boundary condition records. Always specify a small minimum allowed time step, on the order of 1 s. This value may never be used, but it provides the code with flexibility when it may be needed, e.g., when there is a sudden change in boundary fluxes and HYDRUS may not converge with larger time steps.
Maximum Time Step	Maximum permitted value of the time increment, Δt_{max} [T]. This is relatively unimportant parameter and a large value may be specified. Since HYDRUS automatically selects its optimal time step, there is usually no need to constraint that. The only time when there is a need to constrain the time step is likely for cases when HYDRUS is asked to generate internally intra-daily variations in temperature, or in evaporation and transpiration fluxes. Then there is a need to have time step smaller (e.g., 1 h) so that these daily variations can be properly modeled.

3.4. *Output Information*

The **Output Information** dialog window (Fig. 16) contains information governing output from the computational module of HYDRUS.

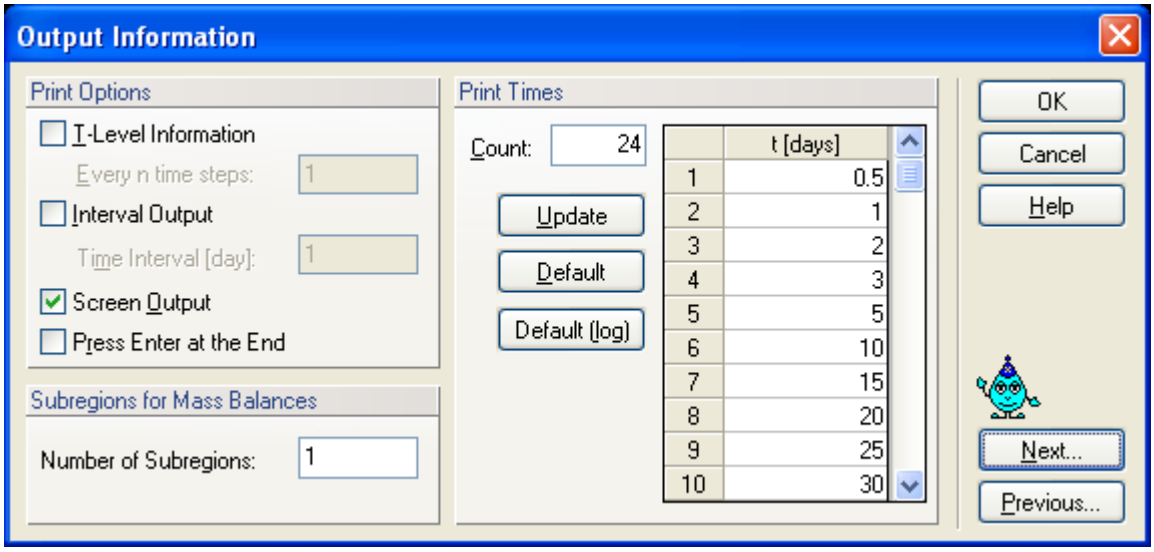


Figure 16. The Output Information dialog window.

In the **Print Options** part of the dialog window, one decides whether certain information concerning mean pressure heads and concentrations, mean water and solute fluxes, cumulative water and solute fluxes, and time and iteration information is printed at each time step (*T-Level Information*), after *n* time steps (*Every n time steps*), at a certain defined time interval (*Interval Output*), or if the information is sent to the screen during the calculations (*Screen Output*). When the simulation ends users are by default asked to hit the Enter key of the keyboard to return to the GUI from the computational window. This action can be disabled by unchecking the Hit Enter at the End check box.

T-Level Information This check box decides whether certain information concerning mean pressure heads and concentrations, mean water and solute fluxes, cumulative water and solute fluxes, and time and iteration information, are to be printed at each time step, after *n* time steps, or only at preselected times (**Print Times**) or **Time Intervals**.

Interval Output Users can specify whether or not information concerning mean pressure heads and concentrations, mean water and solute fluxes, cumulative water and solute fluxes, and time and iteration information is to be printed at a regular **Time Interval**.

Screen Output Check box to decide whether or not information about the simulation run is to be printed to the screen during execution of the HYDRUS computational code. We recommend to check this box for direct problems, but not for inverse problems.

In the **Print Times** part of the dialog window one specifies the number of Print Times (**Count**) at which detailed information about the pressure heads, water contents, concentrations, temperatures, fluxes, and the soil water and solute balances will be printed. Clicking on the **Default** command button will cause the print times to be distributed evenly between the initial and final time. Clicking on the **Default (log)** command button will cause the print times to be distributed evenly between the initial and final time on the log scale. This option is enabled only for larger times.

Finally, in the **Subregions** part one selects the number of regions for which a mass balance will be evaluated and printed to the Balance.out output file.

3.5. *Iteration Criteria*

The **Iteration Criteria** dialog window (Fig. 17) contains information related to the iterative process that is used to solve the Richards equation. Because of the nonlinear nature of the Richards equation, an iterative process must be used to obtain solutions of the global matrix equation at each new time step. For each iteration a system of linearized algebraic equations is first derived and then solved using either Gaussian elimination or the conjugate gradient method. After solving the matrix equation, the coefficients are re-evaluated using this solution, and the new equations are again solved. The iterative process continues until a satisfactory degree of convergence is obtained, i.e., until for all nodes in the saturated (unsaturated) region the absolute change in pressure head (water content) between two successive iterations becomes less than some small value determined by the imposed absolute **Pressure Head** (or **Water Content**) **Tolerance**. The first estimate (at zero iteration) of the unknown pressure heads at each time step is obtained by extrapolation from the pressure head values at the previous two time levels.

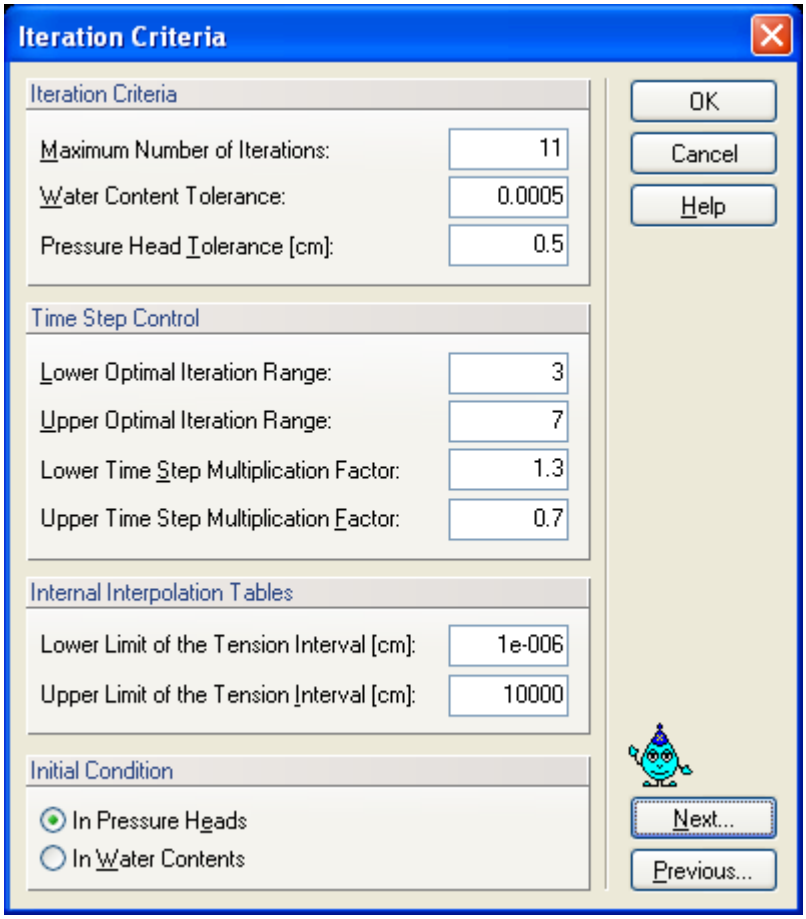


Figure 17. The Iteration Criteria dialog window.

In the **Iteration Criteria** part of the dialog window, one specifies the maximum number of iterations during one time step, and the water content and pressure head precision tolerances.

Max. Number of Iterations Maximum number of iterations allowed during any time step while solving the nonlinear Richards equation using a modified Picard method. The recommended and default value is 10. It is usually not helpful to use a larger value than 10. If HYDRUS does not converge in 10 iterations, then there is a relatively small probability that it will do so during more iteration. Even if it does, it is much more efficient to reduce the time step and attempt to find the solution with a smaller time step, which is done automatically by the program when It_{crit} is reached.

Water Content Tolerance Absolute water content tolerance for nodes in the unsaturated part of the flow region [-]. When the water contents between two successive iterations during a particular time step change less than this parameter, the iterative process stops and the numerical solution proceeds to the new time step. Its recommended and default value is 0.001.

Pressure Head Tolerance Absolute pressure head tolerance for nodes in the saturated part of the flow region [L]. When the pressure heads between two successive iterations during a particular time step change less than this parameter, the iterative process stops and the numerical solution proceeds to the new time step. Its recommended and default value is 1 cm.

Information specified in the **Time Step Control** part of the dialog window is related to the automatic adjustment of the time step during calculations. Four different time discretizations are introduced in HYDRUS: (1) time discretizations associated with the numerical solution, (2) time discretizations associated with implementation of boundary conditions, (3) time discretizations associated with data points used in the inverse problem, and (4) time discretizations which provide printed output of the simulation results (e.g., nodal values of dependent variables, water and solute mass balance components, and other information about the flow regime).

Discretizations 2, 3, and 4 are mutually independent; they generally involve variable time steps as described in the input data file (**Time-Variable Boundary Conditions**, Fig. 37 and **Output Information,** Fig. 16). Discretization 1 starts with a prescribed initial time increment, Δt. This time increment is automatically adjusted at each time level according to the following rules:

a. Discretization 1 must coincide with time values resulting from time discretizations 2, 3, and 4.
b. Time increments cannot become less than a preselected minimum time step, Δt_{min}, nor exceed a maximum time step, Δt_{max} (i.e., $\Delta t_{min} \leq \Delta t \leq \Delta t_{max}$).
c. If, during a particular time step, the number of iterations necessary to reach convergence is ≤3, the time increment for the next time step is increased by multiplying Δt with a predetermined constant >1 (usually between 1.1 and 1.5). If the number of iterations is ≥7, Δt for the next time level is multiplied by a constant <1 (usually between 0.3 and 0.9).
d. If, during a particular time step, the number of iterations at any time level becomes greater than a prescribed maximum (usually between 10 and 50), the iterative process for that time level is terminated. The time step is subsequently reset to $\Delta t/3$, and the iterative process restarted.

We note that the selection of optimal time steps, Δt, during execution is also influenced by the adopted solution scheme for solute transport.

Table 6. Time Step Control variables.

Lower Optimal Iteration Range	When the number of iterations necessary to reach convergence for water flow is less than this number, the time step is multiplied by the lower time step multiplication factor (the time step is increased). Recommended and default value is 3.
Upper Optimal Iteration Range	When the number of iterations necessary to reach convergence for water flow is higher than this number, the time step is multiplied by the upper time step multiplication factor (the time step is decreased). Recommended and default value is 7.
Lower Time Step Multiplication Factor	If the number of iterations necessary to reach convergence for water flow is less than the lower optimal iteration range, the time step is multiplied by this number (time step is increased). Recommended and default value is 1.3.
Upper Time Step Multiplication Factor	If the number of iterations necessary to reach convergence for water flow is higher than the upper optimal iteration range, the time step is multiplied by this number (time step is decreased). Recommended and default value is 0.7.

Internal Interpolation Tables. At the beginning of a numerical simulation, HYDRUS generates for each soil type in the flow domain a table of water contents, hydraulic conductivities, and specific water capacities from the specified set of hydraulic parameters. Values of the hydraulic properties are then computed during the iterative solution process using linear interpolation between entries in the table. If the pressure head h at some node falls outside the prescribed interval (h_a, h_b), the hydraulic characteristics at that node are evaluated directly from the hydraulic functions (i.e., without interpolation). The above interpolation technique was found to be much faster computationally than direct evaluation of the hydraulic functions over the entire range of pressure heads. Interpolation using tables can be avoided by setting h_a and h_b both to zero. Then the soil hydraulic properties are always evaluated directly from the hydraulic functions (i.e., without interpolation). Output graphs of the soil hydraulic properties will be given also for the interval (h_a, h_b).

Lower limit of the tension interval	Absolute value of the lower limit [L] of the pressure head interval for which a table of hydraulic properties will be generated internally for each material.
Upper limit of the tension interval	Absolute value of the upper limit [L] of the pressure head interval for which a table of hydraulic properties will be generated internally for each material.

Finally, in the **Initial Conditions** part of the dialog window, a user specifies whether the initial conditions for the water flow calculations are to be specified in terms of the pressure head or water content.

3.6. *Soil Hydraulic Model*

In the **Soil Hydraulic Model** dialog window (Fig. 18) users select the **Hydraulic Model** to be used to describe the soil hydraulic properties, and specify whether or not **Hysteresis** is to be considered during the calculations.

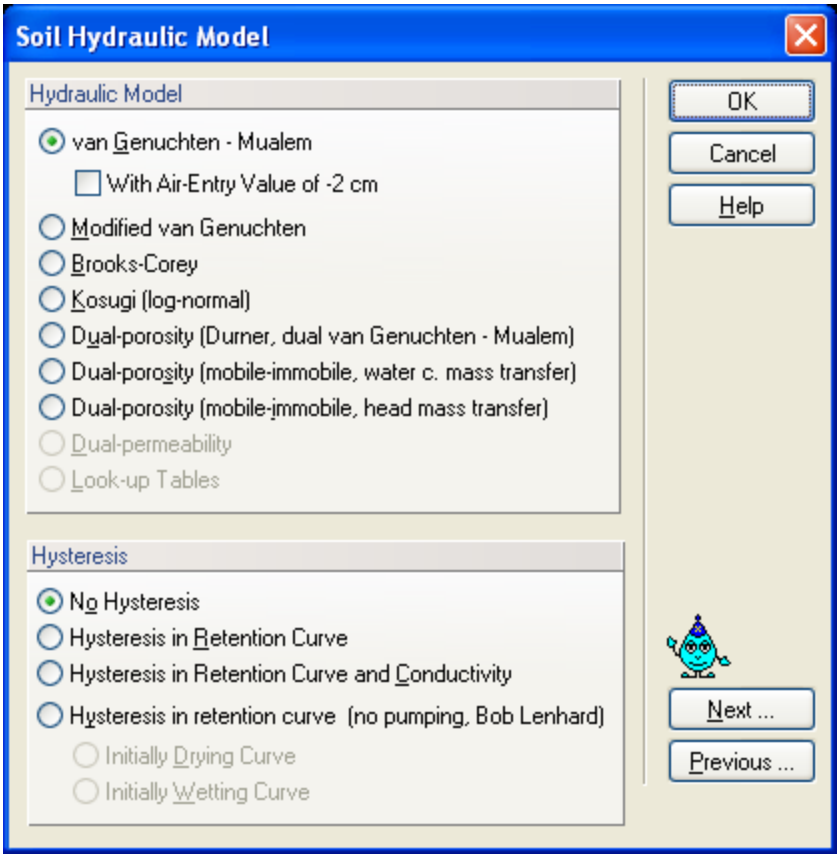


Figure 18. The Soil Hydraulic Model dialog window.

Hydraulic Model: The code allows users to select six types of models for the soil hydraulic properties: a) the van Genuchten-Mualem model [*van Genuchten*, 1980], b) the van Genuchten-Mualem model with an air-entry value of -2 cm, c) the modified van Genuchten type equations [*Vogel and Cislerova*, 1988], d) the equations of *Brooks and Corey* [1964], e) the lognormal distribution model of *Kosugi* [1996], and f) a dual-porosity model [*Durner*, 1994]. Additionally, user can select two dual-porosity nonequilibrium flow models with mass transfer between the mobile and immobile zones assumed to be proportional to either g) the water content or h) the pressure head [*Šimůnek et al.*, 2003]. For a detailed description of these models, see the technical manual of HYDRUS. Two other approaches (a dual-permeability model and look-up tables) are not available in the current version of HYDRUS.

Hysteresis: When the van Genuchten model is used, either a) a non-hysteretic description (*No Hysteresis*), b) a hysteretic description only in the retention curve (*Hysteresis in Retention Curve*), or c) hysteretic descriptions in both the retention curve and the hydraulic conductivity curve (*Hysteresis in Retention Curve and Conductivity*) can be used. When hysteresis in the soil hydraulic properties is assumed, users must specify whether the initial condition is associated with the main wetting (**Initially Wetting Curve**) or main drying (**Initially Drying Curve**) retention curve. The HYDRUS code incorporates hysteresis by using the empirical model introduced by *Scott et al.* [1983]. This model was also employed by *Kool and Parker* [1987], who modified the formulation to account for air entrapment. While relatively simple to implement, the above model has been found to suffer sometimes from a so-called pumping effect, in which the hysteresis loops can move to physically unrealistic parts of the retention function. As an alternative, we also incorporated in HYDRUS the hysteresis model of *Lenhard et al.* [1991] and *Lenhard and Parker* [1992] that eliminates pumping by keeping track of historical reversal points (*Hysteresis in Retention Curve, no pumping, Bob Lenhard*).

3.7. *Water Flow Parameters*

Parameters for the soil hydraulic models are specified in the **Water Flow Parameters** dialog window (Fig. 19).

In all models (i.e., *Brooks and Corey*, 1964; *van Genuchten*, 1980; *Vogel and Cislerova*, 1988; *Kosugi*, 1996, and *Durner*, 1994), θ_r (Qr) and θ_s (Qs) denote the residual and saturated water contents, respectively; K_s (Ks) [LT^{-1}] is the saturated hydraulic conductivity, and l is a pore-connectivity parameter. The parameters α (Alpha) [L^{-1}] and n [-] are empirical coefficients affecting the shape of the hydraulic functions.

The modified van Genuchten model has four additional parameters: θ_a (Qa) – a water content smaller or equal to θ_r, θ_m (Qm) – a water content larger or equal to θ_s, K_k (Kk) [LT^{-1}] – the unsaturated hydraulic conductivity at water content θ_k, and θ_k (Qk) – the water content associated with K_k.

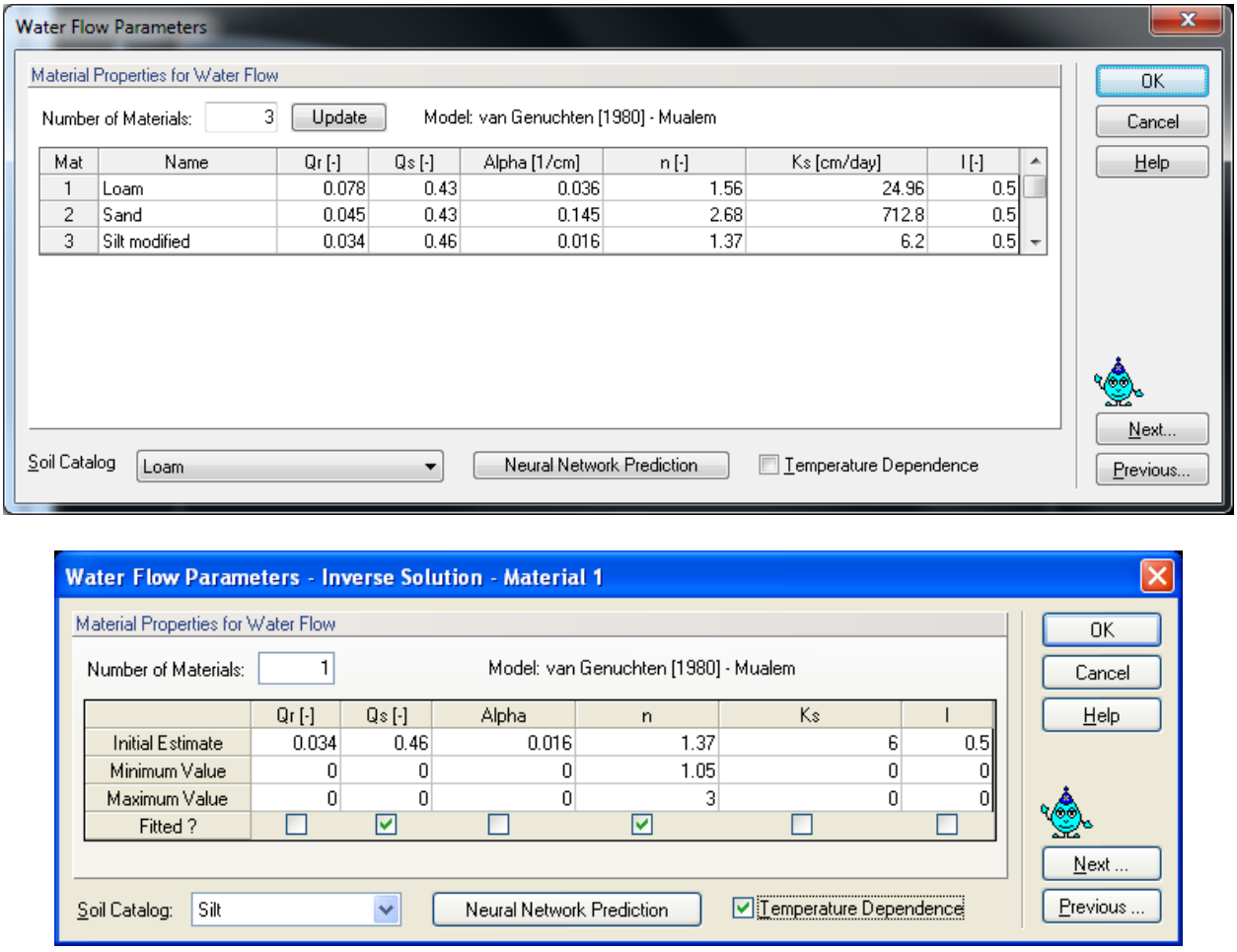

Water Flow Parameters
Material Properties for Water Flow
Number of Materials: 3
Update
Model: van Genuchten [1980] - Mualem
OK
Cancel
Help
Mat | Name | Qr [-] | Qs [-] | Alpha [1/cm] | n [-] | Ks [cm/day] | l [-]
1 | Loam | 0.078 | 0.43 | 0.036 | 1.56 | 24.96 | 0.5
2 | Sand | 0.045 | 0.43 | 0.145 | 2.68 | 712.8 | 0.5
3 | Silt modified | 0.034 | 0.46 | 0.016 | 1.37 | 6.2 | 0.5
Next...
Previous...
Soil Catalog
Loam
Neural Network Prediction
Temperature Dependence
Water Flow Parameters - Inverse Solution - Material 1
Material Properties for Water Flow
Number of Materials: 1
Model: van Genuchten [1980] - Mualem
OK
Cancel
Help
Qr [-] | Qs [-] | Alpha | n | Ks | l
Initial Estimate | 0.034 | 0.46 | 0.016 | 1.37 | 6 | 0.5
Minimum Value | 0 | 0 | 0 | 1.05 | 0 | 0
Maximum Value | 0 | 0 | 0 | 3 | 0 | 0
Fitted ?
Next ...
Previous ...
Soil Catalog:
Silt
Neural Network Prediction
Temperature Dependence

Figure 19. The Water Flow Parameters dialog window for direct (top) and inverse (bottom) problems.

Durner's [1994] model has three additional parameters: w_2 (w2), α_2 (Alpha2) [L^{-1}], and n_2 (n2), where w_2 is the weighting factor for the second overlapping region, and α_2 and n_2 are empirical parameters for the second region.

The hysteretic model has also three additional parameters: θ_{sw} (QsW) – the saturated water content of the main wetting branch, α_w (AlphaW) [L^{-1}] – the shape parameter of the main wetting branch, and K_{sw} (KsW) [LT^{-1}] - the saturated hydraulic conductivity associated with the main wetting branch (in case hysteresis also occurs in the conductivity function).

Temperature Dependence: Check this box if the hydraulic properties are considered to be temperature dependent. Using capillary theory, the influence of temperature on the soil water pressure head is then quantitatively predicted from the influence of temperature on surface tension, while the influence of temperature on the hydraulic conductivity is predicted from the influence of temperature on viscosity and the density of water.

Soil Catalog: The hydraulic parameters of selected soils were included into a catalog from which users can make selections. The parameters were taken from *Carsel and Parrish* [1988] (Table 7). Some caution is needed when using these parameter values since they only represent very approximate averages for different textural classes. The soil hydraulic parameters in the catalog for the Kosugi's model were obtained by fitting retention curves generated using the *Carsel and Parish* [1988] parameters for the *van Genuchten*'s [1980] model using RETC.

The following soil textural classes are represented in the soil hydraulic catalog:

Sand
Loamy Sand
Sandy Loam
Loam
Silt Loam
Sandy Clay Loam
Clay Loam
Silty Clay Loam
Sandy Clay
Silty Clay
Clay

Neural Network Prediction: The program uses pedotransfer functions (PTFs) based on neural networks [*Schaap et al.*, 2001] to predict *van Genuchten*'s [1980] water retention parameters and the saturated hydraulic conductivity (K_s) based on textural information (see Section 3.8 below).

When the parameter estimation option is selected, then users have to provide initial estimates of the optimized soil hydraulic parameters, specify which parameters are to be optimized (check appropriate checkboxes), and provide parameter constraints for the optimization. Entering zeros (the default values) for the minimum and maximum values signifies that the parameters are unconstrained.

Note that in Version 2, each material can have a name (e.g., Material 1, Sand, Clay). When soil hydraulic parameters are assigned using the **Soil Catalog**, the names of textural classes will appear in the **Name** column. These names will then appear throughout the HYDRUS GUI, e.g., at the **Edit Bar** or in the **Sort Property Object** window.

Table 7. Soil hydraulic parameters for the analytical functions of *van Genuchten* [1980] for twelve textural classes of the USDA soil textural triangle according to *Carsel and Parish* [1988].

Textural class	θ_r [L^3L^{-3}]	θ_s [L^3L^{-3}]	α [cm^{-1}]	n [-]	K_s [cm d^{-1}]
Sand	0.045	0.430	0.145	2.68	712.8
Loamy Sand	0.057	0.410	0.124	2.28	350.2
Sandy Loam	0.065	0.410	0.075	1.89	106.1
Loam	0.078	0.430	0.036	1.56	24.96
Silt	0.034	0.460	0.016	1.37	6.00
Silty Loam	0.067	0.450	0.020	1.41	10.80
Sandy Clay Loam	0.100	0.390	0.059	1.48	31.44
Clay Loam	0.095	0.410	0.019	1.31	6.24
Silty Clay Loam	0.089	0.430	0.010	1.23	1.68
Sandy Clay	0.100	0.380	0.027	1.23	2.88
Silty Clay	0.070	0.360	0.005	1.09	0.48
Clay	0.068	0.380	0.008	1.09	4.80

Table 8. Soil hydraulic parameters for the analytical functions of *van Genuchten* [1980] for twelve textural classes of the USDA textural triangle as obtained with the Rosetta Lite program [*Schaap et al.*, 2001].

Textural class	θ_r [L^3L^{-3}]	θ_s [L^3L^{-3}]	α [cm^{-1}]	n [-]	K_s [cm d^{-1}]
Sand	0.053	0.375	0.035	3.18	643.
Loamy Sand	0.049	0.390	0.035	1.75	105.
Sandy Loam	0.039	0.387	0.027	1.45	38.2
Loam	0.061	0.399	0.011	1.47	12.0
Silt	0.050	0.489	0.007	1.68	43.7
Silty Loam	0.065	0.439	0.005	1.66	18.3
Sandy Clay Loam	0.063	0.384	0.021	1.33	13.2
Clay Loam	0.079	0.442	0.016	1.41	8.18
Silty Clay Loam	0.090	0.482	0.008	1.52	11.1
Sandy Clay	0.117	0.385	0.033	1.21	11.4
Silty Clay	0.111	0.481	0.016	1.32	9.61
Clay	0.098	0.459	0.015	1.25	14.8

Table 9. Soil hydraulic parameters for the analytical functions of *Brooks and Corey* [1964] for twelve textural classes of the USDA soil textural triangle according to *Carsel and Parish* [1988].

Textural class	θ_r [L^3L^{-3}]	θ_s [L^3L^{-3}]	α [cm^{-1}]	n [-]	K_s [cm d^{-1}]
Sand	0.020	0.417	0.1380	0.592	504.0
Loamy Sand	0.035	0.401	0.1150	0.474	146.6
Sandy Loam	0.041	0.412	0.0682	0.322	62.2
Loam	0.027	0.434	0.0897	0.220	31.7
Silt	0.015	0.486	0.0482	0.211	16.3
Silty Loam	0.015	0.486	0.0482	0.211	16.3
Sandy Clay Loam	0.068	0.330	0.0356	0.250	10.3
Clay Loam	0.075	0.390	0.0386	0.194	5.52
Silty Clay Loam	0.040	0.432	0.0307	0.151	3.60
Sandy Clay	0.109	0.321	0.0343	0.168	2.88
Silty Clay	0.056	0.423	0.0292	0.127	2.16
Clay	0.090	0.385	0.0268	0.131	1.44

Table 10. Soil hydraulic parameters for the analytical functions of *Kosugi* [1996] for twelve textural classes of the USDA soil textural triangle.

Textural class	θ_r [L^3L^{-3}]	θ_s [L^3L^{-3}]	α [cm^{-1}]	n [-]	K_s [cm d^{-1}]
Sand	0.045	0.430	303.7	0.383	712.8
Loamy Sand	0.057	0.410	12.47	0.950	350.2
Sandy Loam	0.065	0.410	27.42	1.26	106.1
Loam	0.078	0.430	101.8	1.80	24.96
Silt	0.034	0.460	510.6	2.48	6.00
Silty Loam	0.067	0.450	325.9	2.30	10.80
Sandy Clay Loam	0.100	0.390	80.89	2.04	31.44
Clay Loam	0.095	0.410	666.3	2.81	6.24
Silty Clay Loam	0.089	0.430	2853.	3.26	1.68
Sandy Clay	0.100	0.380	1129.	3.41	2.88
Silty Clay	0.070	0.360	140538.	4.49	0.48
Clay	0.068	0.380	103815.	4.67	4.80

3.8. *Neural Network Predictions*

The HYDRUS code was coupled with the Rosetta Lite DLL (Dynamically Linked Library) (Fig. 20), which was independently developed by Marcel Schaap at the U.S. Salinity Laboratory (mschaap@ussl.ars.usda.gov) [*Schaap et al.*, 2001]. Rosetta implements pedotransfer functions (PTFs) which predict *van Genuchten*'s [1980] water retention parameters and the saturated hydraulic conductivity (K_s) in a hierarchical manner from soil textural class, the soil textural distribution, bulk density and one or two water retention points as input. Rosetta has its own help features containing all relevant information and references. Rosetta provides soil hydraulic parameters for the analytical functions of *van Genuchten* [1980] for twelve textural classes of the USDA textural triangle (Table 8).

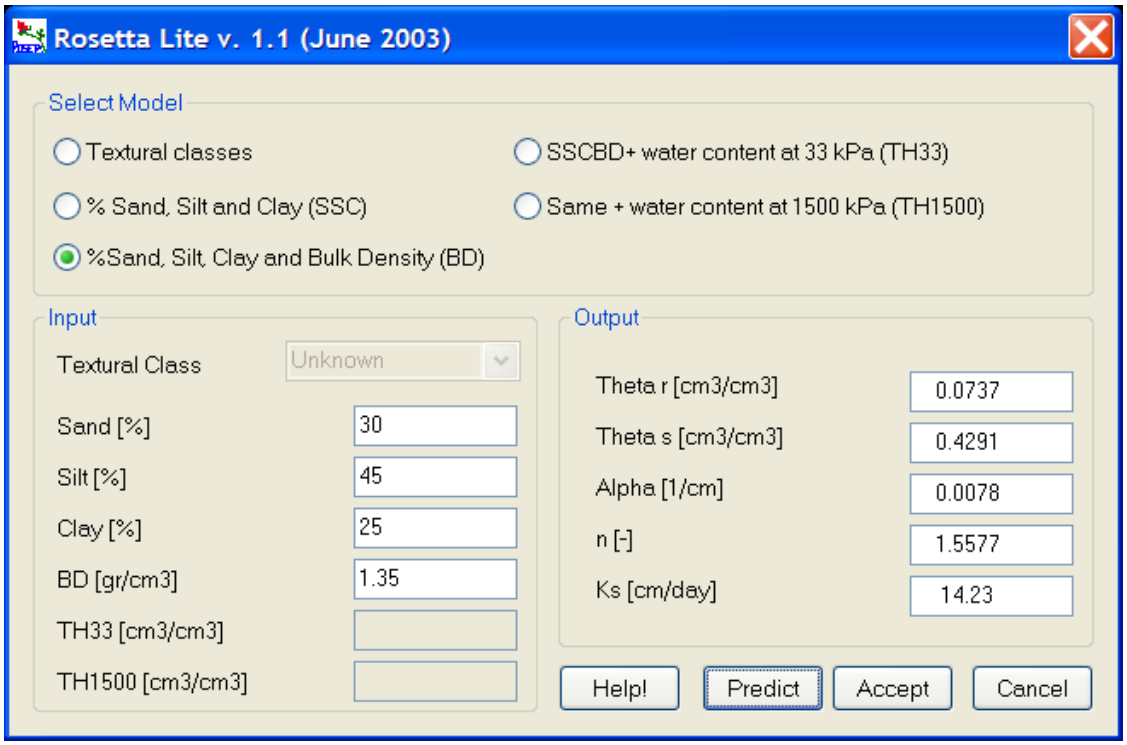


Figure 20. The Rosetta Lite (Neural Network Predictions) dialog window.

3.9. *Anisotropy in the Hydraulic Conductivity*

For two-dimensional problems users may need to specify the principal components of the anisotropy tensor, K_1^A and K_2^A, together with the angle ω_a between the principal direction of K_1^A and the *x*-axis of the global coordinate system for each element (Fig. 21).

Figure 21. The Edit Local Anisotropy dialog window for two-dimensional applications.

This has been simplified for three-dimensional problems where user can specify one or more **Tensors of Anisotropy** (Fig. 22), which may be assigned to different parts of the transport domain. The anisotropy tensor is defined by three principal components, K_1^A (ConAX), K_2^A (ConAY), and K_3^A (ConAZ), and six coefficients a_{ij} that represent the cosine of angles between the *i*th principal direction of the tensor $\boldsymbol{K}^A$ and the *j*-axis of the global coordinate system (i.e., Cos(X-x), Cos(Y-y), Cos(Z-y), Cos(X-y), Cos(X-z), Cos(Y-z)).

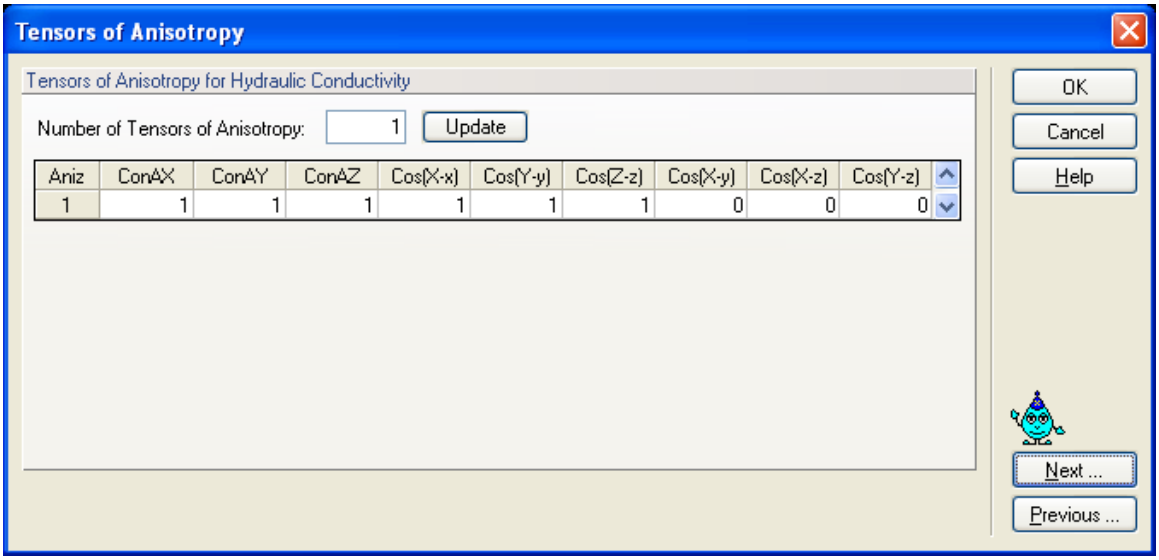


Figure 22. The Tensors of the Anisotropy dialog window.

3.10. *Solute Transport*

Basic information needed for defining solute transport problem are entered in the **Solute Transport** dialog window (Fig. 23). In this window users specify the **Space** and **Time Weighting Scheme**s, the **Iteration Criteria** (for nonlinear problems), and additional **Solute Information** such as mass units, pulse duration (if applicable), and number of solutes.

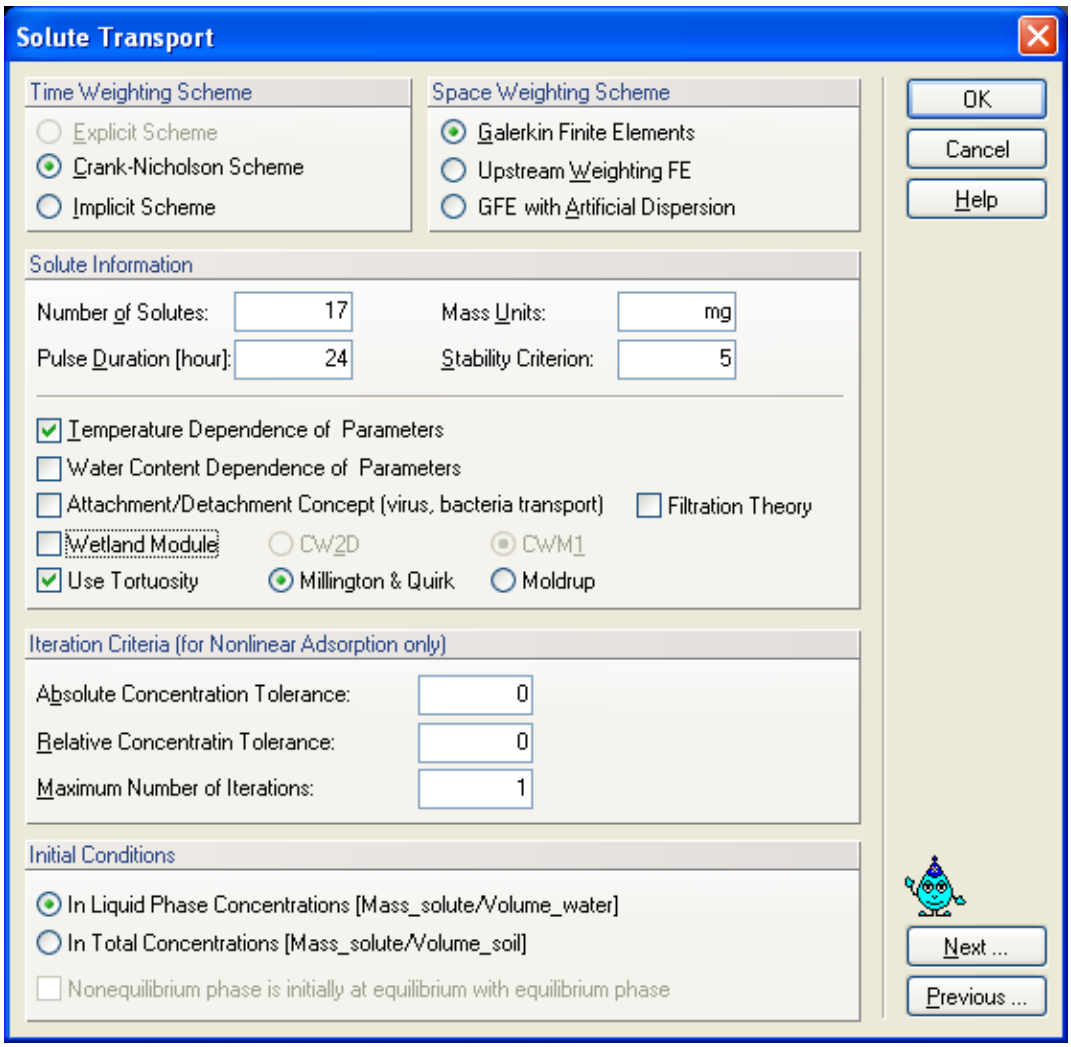


Figure 23. The Solute Transport dialog window.

a) Time Weighting Scheme

The **Time Weighting Scheme** defines the temporal weighing coefficient, ε, used in the numerical solution of the transport equation. The temporal weighting coefficient is equal to 0.0 for an *explicit scheme*, 0.5 for a *Crank-Nicholson time-centered implicit scheme*, and 1.0 for a *fully implicit scheme*. The structure of the final set of linear equations [G] {c} = {g}, obtained after the spatial and temporal discretization of the governing advection-dispersion equation, depends upon the value of the temporal weighing factor, ε. The explicit (ε=0) and fully implicit (ε=1) schemes

require that the global matrix [*G*] and the vector {*g*} be evaluated at only one time level (the previous or current time level). The other two schemes require evaluation at both time levels. Also, the Crank-Nicholson and implicit schemes lead to an asymmetric banded matrix [*G*]. By contrast, the explicit scheme (ε=0) leads to a diagonal matrix [*G*] which is much easier to solve (but generally requires much smaller time steps).

The Crank-Nicholson centered scheme is recommended in view of solution precision. The fully implicit scheme also leads to numerical dispersion, but is better in avoiding numerical instabilities. The explicit scheme is most prone to numerical instabilities with undesired oscillations (and is currently disabled).

b) Space Weighting Scheme

HYDRUS provides three options for the **Space Weighting Scheme**, i.e., the regular *Galerkin Finite Elements* formulation, the *Upstream Weighting Finite Elements* formulation, and the *Galerkin Finite Elements* formulation *with Artificial Dispersion*.

While the **Galerkin Finite Elements** formulation is recommended in view of solution precision, **Upstream Weighting** is provided as an option in HYDRUS to minimize some of the problems with numerical oscillations when relatively steep concentration fronts are being simulated. For this purpose the second (flux) term of advective-dispersive equation is not weighted by regular linear basis functions, but instead using nonlinear functions [*Yeh and Tripathi*, 1990]. The weighing functions ensure that relatively more weight is placed on flow velocities of nodes located at the upstream side of an element.

Additional **Artificial Dispersion** may be added also to stabilize the numerical solution and to limit or avoid undesired oscillations in the Galerkin finite element results. Artificial dispersion is added such that a **Stability Criterion** involving Pe.Cr (the product of the Peclet number and the Curant number) [*Perrochet and Berod*, 1993] is satisfied. The recommended value for Pe.Cr is 2.0.

c) Solute Information

Number of Solutes — Number of solutes to be simulated simultaneously or involved in a decay chain reaction.

Pulse Duration — Time duration of the concentration pulse. Concentrations (flux or resident) along all boundaries, for which no time-variable boundary conditions are specified, are then set equal to zero for times larger than the "Pulse Duration".

Mass Units — Units to be printed to the output files or displayed in various graphs. Mass units have no effect on the calculations. Concentration units in general should be given in [ML^{-3}], where M is **Mass Units** specified in the **Solute Transport** dialog window (Fig. 22) and L is **Length Units** specified in the **Domain Type and Units** dialog window (Fig. 6). However, since the concentration variable appears in each term of the governing solute

transport equations (Eq. 3.1 and 3.2 of the Technical Manual), it is possible to use different length units than those used to define geometry and fluxes (e.g., geometry may be specified in meters while concentrations are given in mg/cm^3). In such case the solute fluxes (cq) will then be in units of $ML_c^{-3}L_gT^{-1}$ where L_c is the length unit (e.g. cm) used to define concentrations and L_g the length unit defining geometry and fluxes (e.g., m). Similarly the solute mass ($c\theta V$) obtained by integrating solute over the transport domain will be in units of $ML_c^{-3}L_g^2$. Similar adjustments of units need to be done for other variables that involve both concentration and length units.

Stability Criterion Product of the dimensionless Peclet and Curant numbers (Pe.Cr). This criterion is used either to add artificial dispersion in the *Galerkin Finite Elements with Artificial Dispersion* scheme or to limit the time step (leading to lower Courant numbers for a given Peclet number) for the *Galerkin Finite Elements* scheme.

Use Tortuosity Factor Check this box when molecular diffusion coefficients in the water and gas phases are to be multiplied by a tortuosity factor according to the formulation of either *Millington and Quirk* [1991] or *Moldrup et al.* [1997, 2000].

Temperature Dependence Check this box if the solute transport and reaction parameters are assumed to be temperature dependent.

Water Content Dependence Check this box if the solute reaction parameters are assumed to be water content dependent [*Walker*, 1974].

Attachment/Detachment Check this box if the solute is assumed to be subject to attachment/detachment to/from the solid phase. This process is often used in simulations of the transport of viruses, colloids, or bacteria.

Filtration Theory Check this box if the attachment coefficient is to be calculated from filtration theory.

Wetland Module Check this box if the Wetland module is to be used. The Wetland module (for two-dimensional problems only) was developed to model biochemical transformation and degradation processes in subsurface flow constructed wetlands. In the wetland module two biokinetic model formulations can be chosen: (1) the biokinetic model as described in CW2D [*Langergraber and Šimunek*, 2005, 2006] and (2) the CWM1 (Constructed Wetland Model #1) biokinetic model [*Langergraber et al.*, 2009]. In CW2D aerobic and anoxic transformation and degradation processes for organic matter, nitrogen and phosphorus are described, whereas in CWM1 aerobic, anoxic and anaerobic processes for organic matter, nitrogen and sulphur.

d) Iteration Criteria

The advection-dispersion solute transport equation becomes nonlinear when nonlinear adsorption is considered. Similarly as for the Richards equation, an iterative process must then be used to obtain solutions of the global matrix equation at each new time step. During each iteration a system of linearized algebraic equations is derived and solved using either Gaussian elimination or the conjugate gradient method. After inversion, the coefficients are re-evaluated using the initial solution, and the new equations are again solved. This iterative process continues until a satisfactory degree of convergence is obtained, i.e., until at all nodes the absolute change in concentration between two successive iterations becomes less than some concentration tolerance (defined in HYDRUS as the sum of an **Absolute Concentration Tolerance** and the product of the concentration and a **Relative Concentration Tolerance** (the recommended and default value is 0.001)). The **Maximum Number of Iterations** allowed during a certain time step needs to be specified (recommended value is 10). When the **Maximum Number of Iterations** is reached then the numerical solution is either (a) terminated for problems involving transient water flow or (b) restarted with a reduced time step for steady-state flow problems.

e) Initial Conditions

Initial Conditions can be specified either using liquid phase concentrations in units of mass of solute [M_c] per volume of water [$M_c L_w^{-3}$] or using total concentrations in units of mass of solute per volume of soil [$M_c L_s^{-3}$]. In the latter case the liquid phase concentration is calculated from the total concentration depending on the distribution coefficients (e.g., K_d, or Henry's constant) between different phases.

Rather then specifying directly the initial values of the nonequilibrium phase concentrations (e.g., concentrations in the immobile water for the dual-porosity models or concentrations kinetically sorbed to the solid phase for the two-site sorption models, or for concentrations associated with the solid phase for the attachment/detachment models), users can specify that the nonequilibrium phase concentrations are initially at equilibrium with the equilibrium phase concentrations. Initial conditions need to be then specified only for the liquid phase concentrations, and the nonequilibrium phase concentrations are calculated by HYDRUS.

The UNSATCHEM Module

When the UNSATCHEM module is used, basic information needed for defining solute transport problem are entered in the **Solute Transport** dialog window displayed in Figure 24 (instead of Figure 23, which is used for the standard solute transport module). In this window users specify again the **Space** and **Time Weighting Scheme**s, and additional **Solute Information** such as mass units. Note that all concentrations in the UNSATCHEM module are either in meq/L (in the liquid phase) or meq/kg (in the solid phase) (meq=$mmol_c$). The pulse duration is not used in UNSATCHEM and the number of solutes is fixed to 8 (i.e., the number of considered major ions: Ca^{2+}, Mg^{2+}, Na^+, K^+, Alkalinity, SO_4^{2-}, Cl^-, and an independent tracer). The number of solution, adsorbed, and precipitated concentration combinations is specified when simulating the transport of major ions in the UNSATCHEM module. This value represents the maximum

number of (solution, adsorbed, and precipitated) concentration combinations, which can be used to specify the initial and boundary conditions.

Since there is currently no technical manual describing the two-dimensional version of the UNSATCHEM module, users are referred to the HYDRUS-1D manual [*Šimůnek et al.,* 2008], which provides all relevant information about this module.

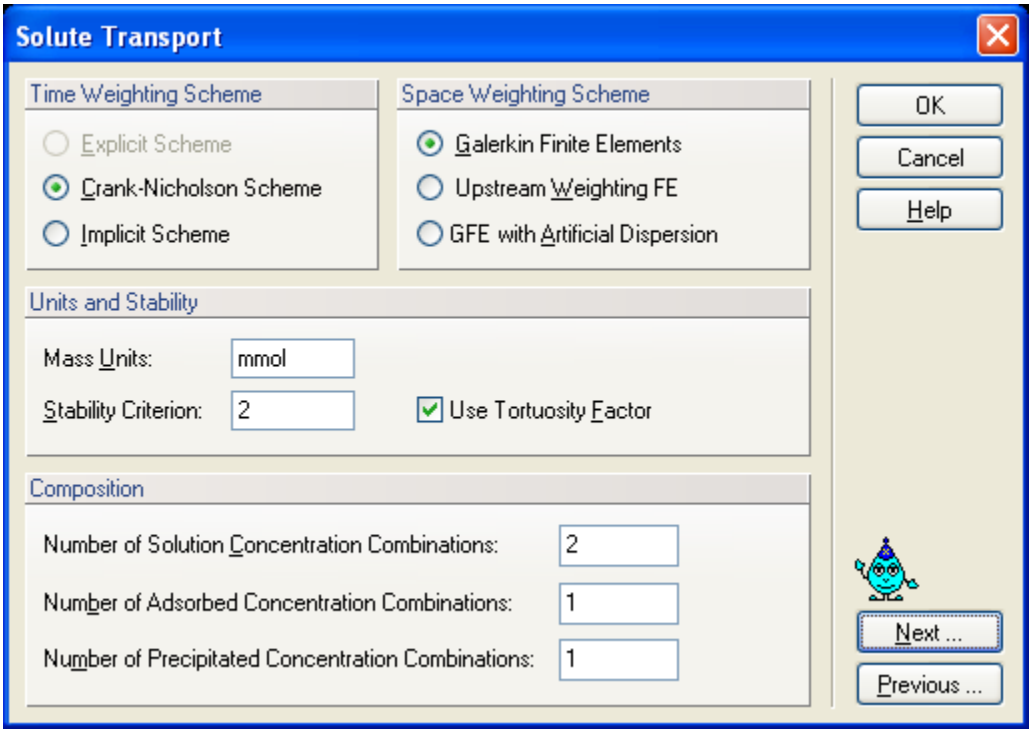


Figure 24. The Solute Transport dialog window for the UNSATCHEM module.

3.11. *Solute Transport Parameters*

Soil and *Solute Specific Transport Parameters* are specified in the **Solute Transport Parameters** dialog window (Fig. 25).

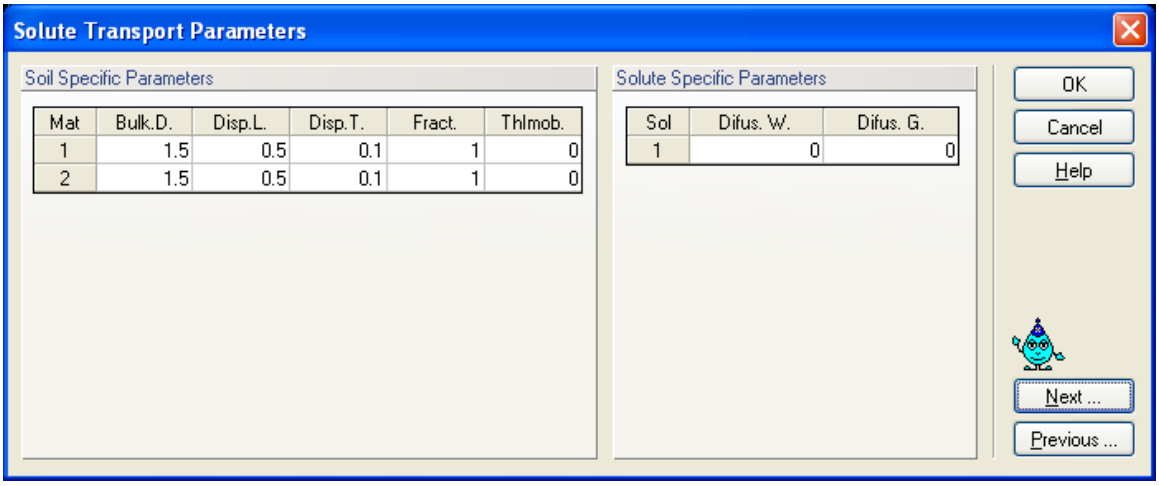


Figure 25. The Solute Transport Parameters dialog window.

The following **Soil Specific Parameters** (left part of the dialog window) are specified for each soil material:

Bulk.d. Bulk density, ρ [ML^{-3}]
Disp.L. Longitudinal dispersivity, D_L [L]
Disp.T. Transverse dispersivity, D_T [L]
Frac Dimensionless fraction of adsorption sites classified as type-1 sites, i.e., sites with instantaneous sorption when the **chemical nonequilibrium** option is considered [-]. Set this parameter equal to 1 when equilibrium transport is considered. *Frac* becomes the dimensionless fraction of adsorption sites in contact with mobile water when the **physical nonequilibrium** option is considered [-]. In that case *Frac* should be set equal to 1 when all sorption sites are in contact with mobile water.
ThImob The immobile water content. Set equal to 0 when the **physical nonequilibrium** option is not considered.

The following **Solute Specific Parameters** (right part of the dialog window) are specified for each solute:

Diffus.W Molecular diffusion coefficient in free water, D_w [L^2T^{-1}]
Diffus.G Molecular diffusion coefficient in soil air, D_a [L^2T^{-1}]

3.12. *Solute Reaction Parameters*

The *Solute Reaction Parameters* and concentrations for *Boundary Conditions* are specified in the **Solute Reaction Parameters** dialog window (Fig. 26). Each solute has its own Solute Reaction Parameters dialog window.

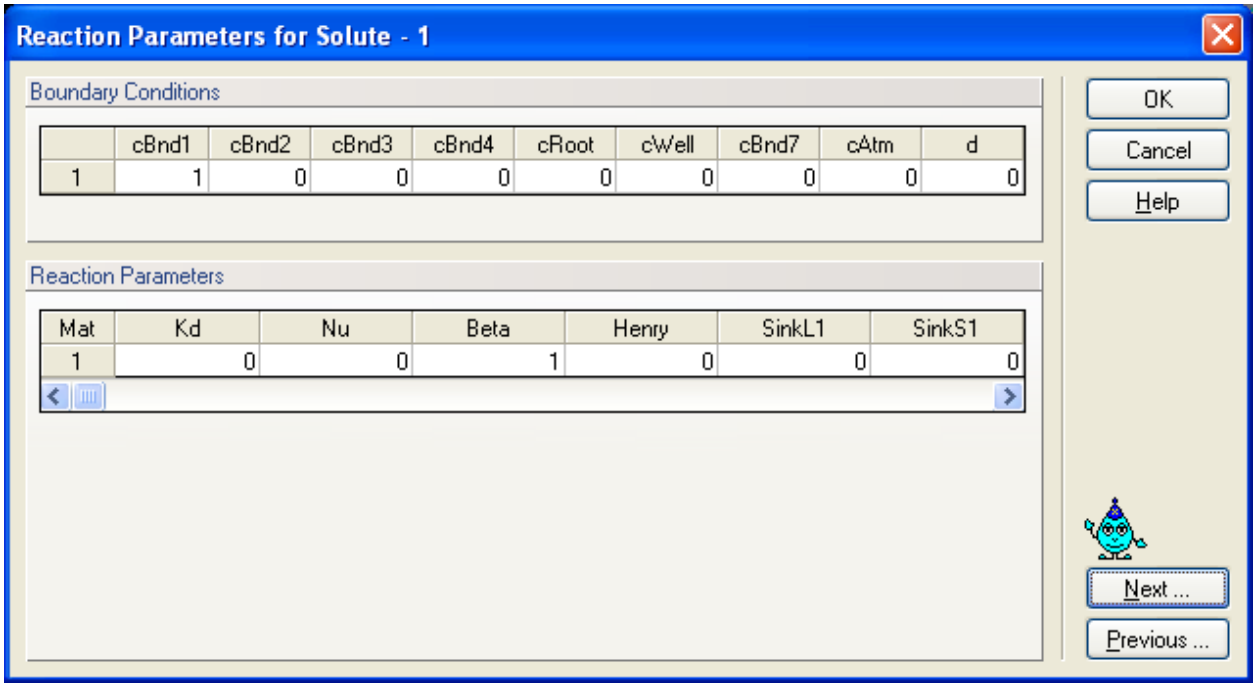

Reaction Parameters for Solute - 1
Boundary Conditions
cBnd1 cBnd2 cBnd3 cBnd4 cRoot cWell cBnd7 cAtm d
1 1 0 0 0 0 0 0 0 0
Reaction Parameters
Mat Kd Nu Beta Henry SinkL1 SinkS1
1 0 0 1 0 0 0
OK
Cancel
Help
Next ...
Previous ...

Figure 26. The Solute Reaction Parameters dialog window.

The following **Solute Reaction Parameters** are specified for each soil material:

Kd	Adsorption isotherm coefficient, k_s [$M^{-1}L^3$]
Nu	Adsorption isotherm coefficient, η [$M^{-1}L^3$]
Beta	Adsorption isotherm exponent, β [-]
Henry	Equilibrium distribution constant between liquid and gaseous phases, k_g [-]
SinkL1	First-order rate constant for dissolved phase, μ_w [T^{-1}]
SinkS1	First-order rate constant for solid phase, μ_s [T^{-1}]
SinkG1	First-order rate constant for gas phase, μ_g [T^{-1}]
SinkL1'	First-order rate constant for dissolved phase, μ_w' [T^{-1}], as part of a solute decay chain
SinkS1'	First-order rate constant for solid phase, μ_s' [T^{-1}], as part of a solute decay chain
SinkG1'	First-order rate constant for gas phase, μ_g' [T^{-1}], as part of a solute decay chain
SinkW0	Zero-order rate constant for dissolved phase, γ_w [$ML^{-3}T^{-1}$]
SinkS0	Zero-order rate constant for solid phase, γ_w [T^{-1}]
SinkG0	Zero-order rate constant for gas phase, γ_s [$ML^{-3}T^{-1}$]

Alpha First-order rate coefficient for one-site or two-site nonequilibrium adsorption, mass transfer coefficient for solute exchange between mobile and immobile liquid regions, ω[T^{-1}]

When the **Attachment/Detachment Model** (Fig. 23) is used, then some parameters listed above are replaced with different parameters needed for the attachment/detachment model:

D_Soil Diameter of the sand grains, d_c [L]. Note that HYDRUS allow only one value (for all materials) and that this value is used only in the Depth-dependent blocking function (iPsi=4) developed by *Bradford et al.* [2002], which was developed for homogeneous laboratory column. It is less clear have is should be used in multi-layered systems (for other than the first layer). Also note that this blocking function depends on a vertical spatial coordinate. This means that one needs to specify the origin of the function, i.e., the inflow and inter-material interfaces. HYDRUS allows doing this for up to 2 materials using the cBnd vector as described in the help.

iPsi2 Type of blocking on the second sorption sites:
= 0: No blocking.
= 1: Langmuirian dynamics.
= 2: Ripening.
= 3: random sequential adsorption model.
= 4: depth dependent blocking coefficient.

iPsi1 Same for the first sorption sites.

SMax2 Parameter in the blocking function for the second sorption sites (s_{max} for blocking options (1), (2) and (3), and *b* for (4)).

AttachSolid2 First-order deposition (attachment) coefficient, k_a [T^{-1}], for the second sorption sites.

DetachSolid2 First-order entrainment (detachment) coefficient, k_d [T^{-1}], for the second sorption sites.

SMax1 Parameter in the blocking function for the first sorption sites.

AttachSolid1 First-order deposition (attachment) coefficient, k_a [T^{-1}], for the first sorption sites.

DetachSolid1 First-order entrainment (detachment) coefficient, k_d [T^{-1}], for the first sorption sites.

When **Filtration Theory** (Fig. 23) is used to calculate the attachment coefficient, then the following parameters must be entered instead:

D_Soil Diameter of the sand grains, d_c [L].

D_Virus Diameter of the particle, d_p (e.g., virus, bacteria) (e.g., = 0.95 μm or 0.95e-6 m) [L].

SMax2 Parameter in the blocking function for the second sorption sites (s_{max} for model (1)).

Stick. Eff2 Sticking efficiency, *a* [-], for the second sorption sites.

DetachSolid2 First-order entrainment (detachment) coefficient, k_d [T^{-1}], for the second sorption sites.

SMax1 Parameter in the blocking function for the first sorption sites.
Stick. Eff1 Sticking efficiency, *a* [-], for the first sorption sites.
DetachSolid1 First-order entrainment (detachment) coefficient, k_d [T^{-1}], for the first sorption sites.

Boundary Conditions:
Concentrations for time-independent Boundary Conditions are also specified in this dialog window.

cBnd1 Value of the concentration for the first time-independent boundary condition [ML^{-3}]. Set equal to zero if no time-independent boundary condition is specified. The same for cBnd2 through cBnd4

cRoot Value of the concentration for the fifth time-independent boundary condition [ML^{-3}]. If water uptake is considered then *cRoot* is automatically used for the maximum concentration of water removed from the flow region by root water uptake. When zero is specified, then all solute is left behind in the soil and only a solute-free solution is being taken up. When the concentration is lower than *cRoot*, all solute is taken up. When the concentration is higher than *cRoot*, the excess solute stays behind. Set equal to zero if no fifth time-independent boundary condition and no solute uptake by roots is considered.

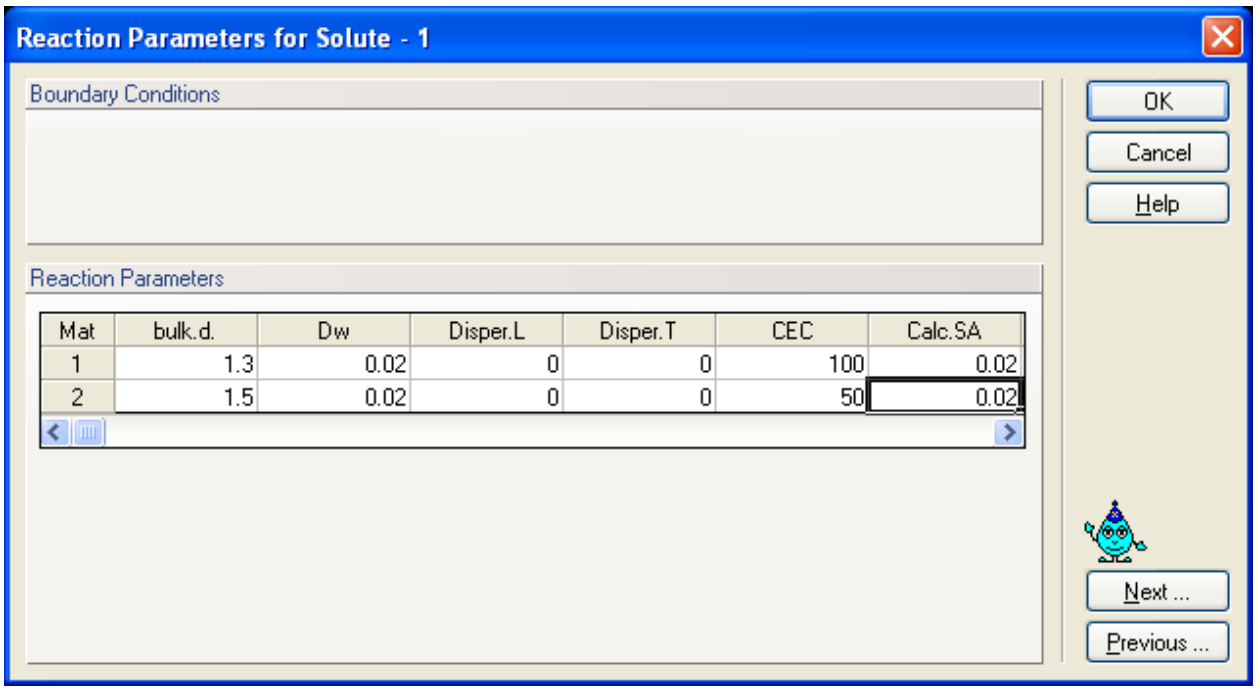
cWell Value of the concentration for the sixth time-independent boundary condition [ML^{-3}]. If internal sources are specified, then *cWell* is automatically used for the concentration of water injected into the flow region through internal sources. Set equal to zero if no sixth time-independent boundary condition and no internal sources are specified.

cBnd7 Concentration of the incoming fluid for a volatile type boundary condition at the soil surface [ML^{-3}]. Set equal to zero if no volatile boundary condition is specified.

cAtm Concentration above the stagnant boundary layer, g_{atm} [ML^{-3}], for a volatile type boundary condition. Set equal to zero if no volatile boundary condition is being specified.

d Thickness of the stagnant boundary layer, *d* [L], for a volatile type boundary condition. Set equal to zero if no volatile boundary condition is being specified.

When the parameter estimation option is selected, then users have to provide initial estimates of the optimized solute transport parameters, specify which parameters are to be optimized (select appropriate checkboxes), and provide parameter constraints for the optimization. Zero values for minimum and maximum values signify that the parameters are unconstrained. The **Solute Transport and Reaction Parameters** dialog window for the inverse problem is not further shown here.



Mat	bulk.d.	Dw	Disper.L	Disper.T	CEC	Calc.SA
1	1.3	0.02	0	0	100	0.02
2	1.5	0.02	0	0	50	0.02

Figure 27. The Solute Reaction Parameters dialog window for the UNSATCHEM module.

The UNSATCHEM Module

When the UNSATCHEM module is used, the *Solute Reaction* (and *transport*) *Parameters* are specified in the **Solute Reaction Parameters** dialog window displayed in Figure 27 (instead of Figure 26, which is used for the standard solute transport module). The following **Soil Specific Parameters** are specified for each soil material:

Bulk.d. Bulk density, ρ [ML^{-3}]
Dw Molecular diffusion coefficient in free water, D_w [L^2T^{-1}]
Disper.L. Longitudinal dispersivity, D_L [L]
Disper.T. Transverse dispersivity, D_T [L]
CEC Cation exchange capacity, CEC [meq/kg]
Calc.SA Calcite surface area [m^2/dm^3]
Dol.SA Dolomite surface area [m^2/dm^3]
DOC Dissolved organic carbon [$mmol/dm^3$]
K[Ca/Mg] Gapon constant for exchange of calcium and magnesium
K[Ca/Na] Gapon constant for exchange of calcium and sodium
K[Ca/K] Gapon constant for exchange of calcium and potassium

3.13. *Temperature Dependence of Solute Reaction Parameters*

Several of the diffusion (D_w, D_g), zero-order production (γ_w, γ_s, γ_g), first-order degradation (μ_w', μ_s', μ_g', μ_w, μ_s, and μ_g), and adsorption (k_s, k_g, β, η, ω) coefficients may be strongly dependent upon temperature. HYDRUS assumes that this dependency can be expressed by the Arrhenius equation [*Stumm and Morgan*, 1981]. This equation can be expressed in the general form

$$a_T = a_r \exp\left[\frac{E_a(T^A - T_r^A)}{R_u T^A T_r^A}\right]$$

where a_r and a_T are values of the coefficient being considered at a reference absolute temperature T_r^A and absolute temperature T^A, respectively; R_u is the universal gas constant, and E_a [$ML^2T^{-2}M^{-1}$] is the activation energy of the particular reaction or process being modeled.

The activation energy characterizing the temperature dependence of the solute transport and reaction parameters is entered in the dialog window shown in Figure 28.

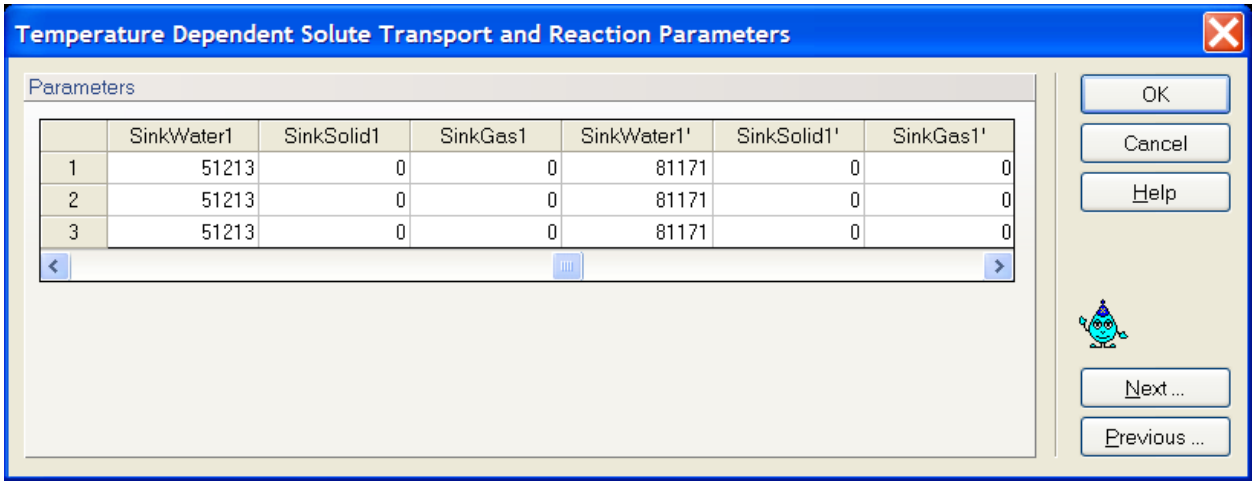


Figure 28. The Temperature Dependent Solute Transport and Reaction Parameters dialog window.

3.14. *Water Content Dependence of Solute Reaction Parameters*

The water content dependence of degradation coefficients is implemented using a modified equation of *Walker* [1974]:

$$\mu(\theta) = \mu_r(\theta_r)\min\left[1, \left(\frac{\theta}{\theta_r}\right)^B\right]$$

where μ_r is the values of a particular coefficient (rate constant) at the reference water content θ_r, μ is the value of this coefficient at the actual water content θ, and B is a solute dependent parameter (usually 0.7). The reference water content, θ_r, which may be different for different soil layers, is calculated from the reference pressure head, h_r, which is considered to be constant for a particular compound. The solute dependent exponent, B, and the reference pressure head, h_r, are entered in the **Water Content Dependent Solute Reaction Parameters** dialog window shown in Figure 29.

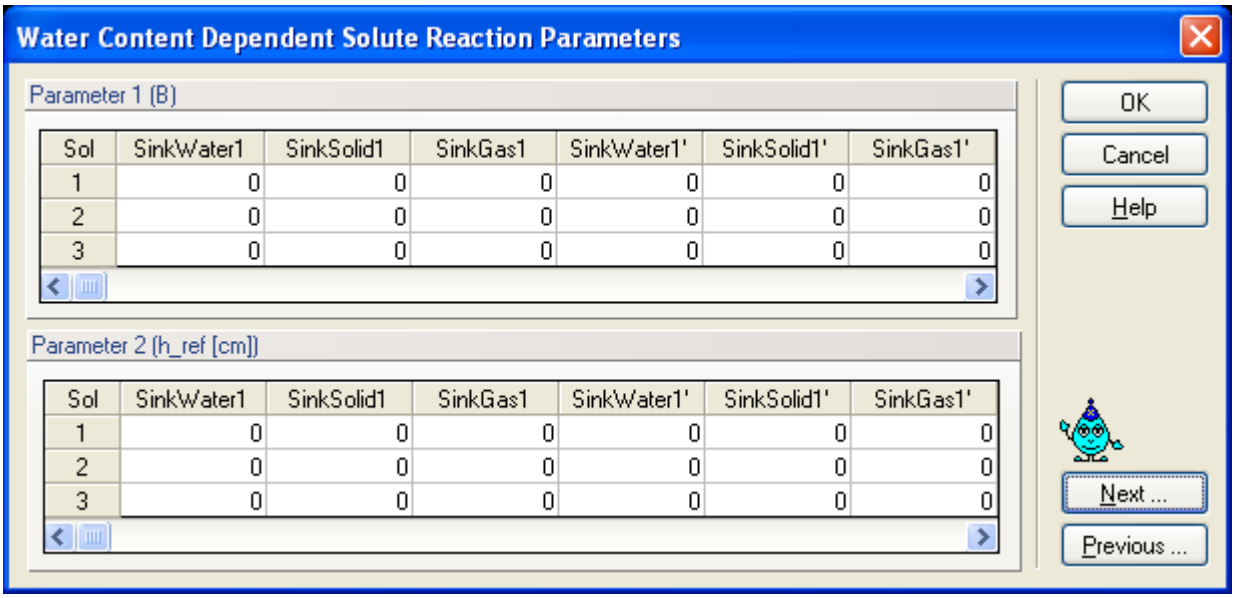

Water Content Dependent Solute Reaction Parameters
Parameter 1 (B)
Sol SinkWater1 SinkSolid1 SinkGas1 SinkWater1' SinkSolid1' SinkGas1'
1 0 0 0 0 0 0
2 0 0 0 0 0 0
3 0 0 0 0 0 0
Parameter 2 (h_ref [cm])
Sol SinkWater1 SinkSolid1 SinkGas1 SinkWater1' SinkSolid1' SinkGas1'
1 0 0 0 0 0 0
2 0 0 0 0 0 0
3 0 0 0 0 0 0
OK
Cancel
Help
Next ...
Previous ...

Figure 29. The Water Content Dependent Solute Reaction Parameters dialog window.

3.15. *Solution Compositions for the UNSATCHEM Module*

The set of solution, adsorbed, and precipitated concentration combinations for the UNSATCHEM module is specified in the **Solution Compositions** dialog window (Fig. 30). These (solution, adsorbed, and precipitated) concentration combinations can be used to specify the initial and boundary conditions. The number of solution, adsorbed, and precipitated concentration combinations is specified in the **General Solute Transport Information** window (Fig. 24). **Solution Concentrations** need to be specified for all major ions: Ca^{2+}, Mg^{2+}, Na^{+}, K^{+}, Alkalinity, SO_4^{2-}, Cl^{-}, and an independent tracer; **Adsorbed Concentrations** for all cations: Ca^{2+}, Mg^{2+}, Na^{+}, and K^{+}; and **Precipitated Concentrations** for all solids that UNSATCHEM can consider: calcite, dolomite, gypsum, nesquohonite, hydromagnesite, and sepiolite. **Solution Concentrations** need to be specified in meq/L (L = liter), and **Adsorbed Concentrations** and **Precipitated Concentrations** in meq/kg (meq=$mmol_c$).

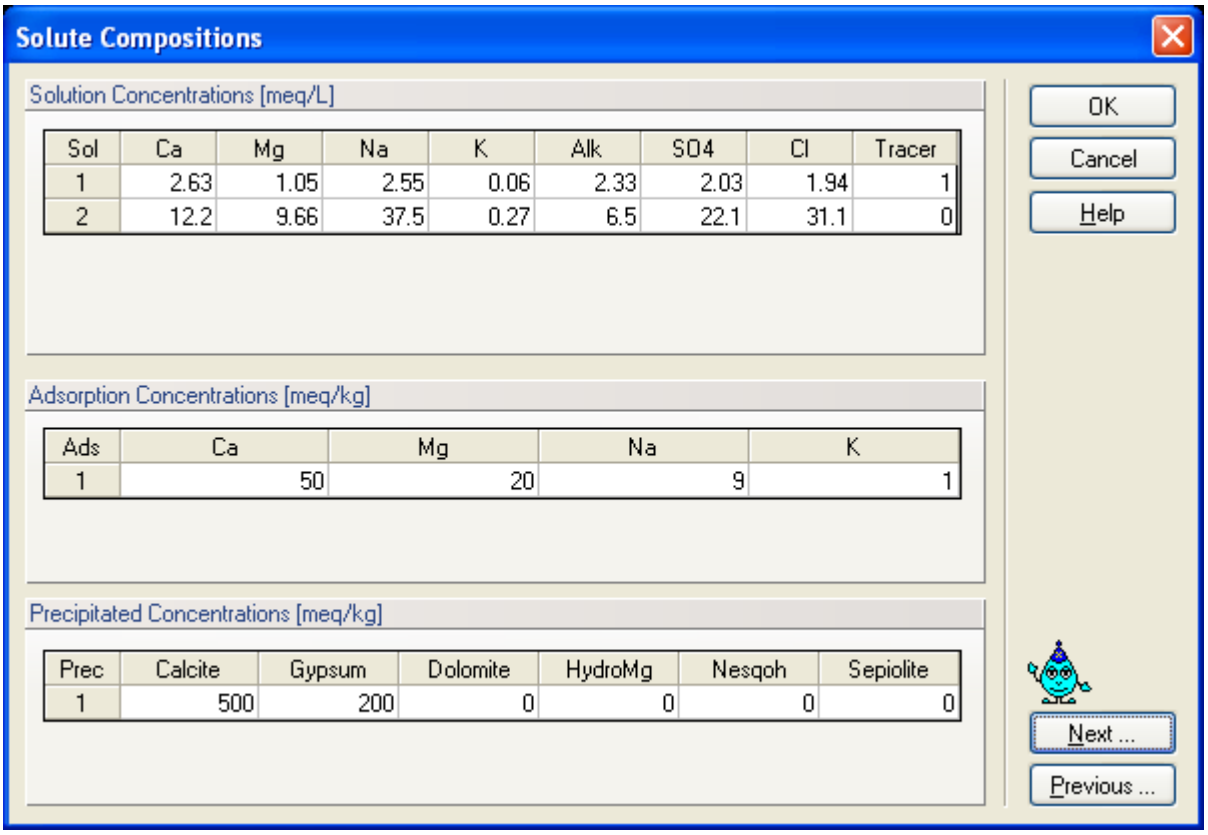

Solute Compositions
Solution Concentrations [meq/L]
Sol Ca Mg Na K Alk SO4 Cl Tracer
1 2.63 1.05 2.55 0.06 2.33 2.03 1.94 1
2 12.2 9.66 37.5 0.27 6.5 22.1 31.1 0
Adsorption Concentrations [meq/kg]
Ads Ca Mg Na K
1 50 20 9 1
Precipitated Concentrations [meq/kg]
Prec Calcite Gypsum Dolomite HydroMg Nesqoh Sepiolite
1 500 200 0 0 0 0
OK
Cancel
Help
Next ...
Previous ...

Figure 30. The Solution Compositions dialog window for the UNSATCHEM module.

3.16. *Chemical Parameters for the UNSATCHEM module.*

The following chemical parameters and selections for the UNSATCHEM module are specified in the **Chemical Parameters** dialog window (Fig. 31):

- Whether the kinetic or equilibrium model for the precipitation and dissolution of calcite and dissolution of dolomite is to be used (the **Kinetic Precipitation/Dissolution** check box).
- Whether the silica content in the solution is to be calculated based on the solution pH, or whether the effect of pH is to be neglected (the **Silica in Solution (pH Dependency)** check box).
- The **Critical Ionic Strength**, i.e., the ionic strength, below which the extended Debye-Hückel equation is used to calculate ion activity coefficients. Pitzer virial-type equations are used above this value.
- The **Maximum Number of Iterations** allowed during any time step between the solute transport and chemical modules. When the maximum number of iterations is reached then the code proceeds to the new time level. The recommended value (if the iterative approach is to be used; from our experience) is 5. Set equal to one if no iteration (we recommend this non-iterative approach) is required (this, in general, leads to significantly lower computational time without significantly altering the results in most cases).
- Whether the hydraulic conductivity is to be modified depending on the solution chemistry using the *McNeal* [1968] semi-empirical approach (the **Conductivity Reduction due to Chemistry** check box).

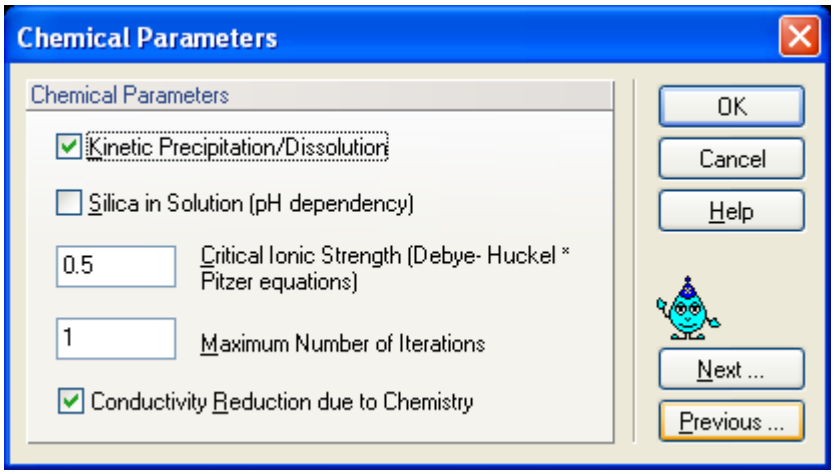


Figure 31. The Chemical Parameters dialog window for the UNSATCHEM module.

3.17. *Heat Transport Parameters*

Information needed for defining heat transport problem is entered in the **Heat Transport** dialog window (Fig. 32). In this window users specify *Heat Transport Parameters* and temperatures for the *Boundary Conditions*.

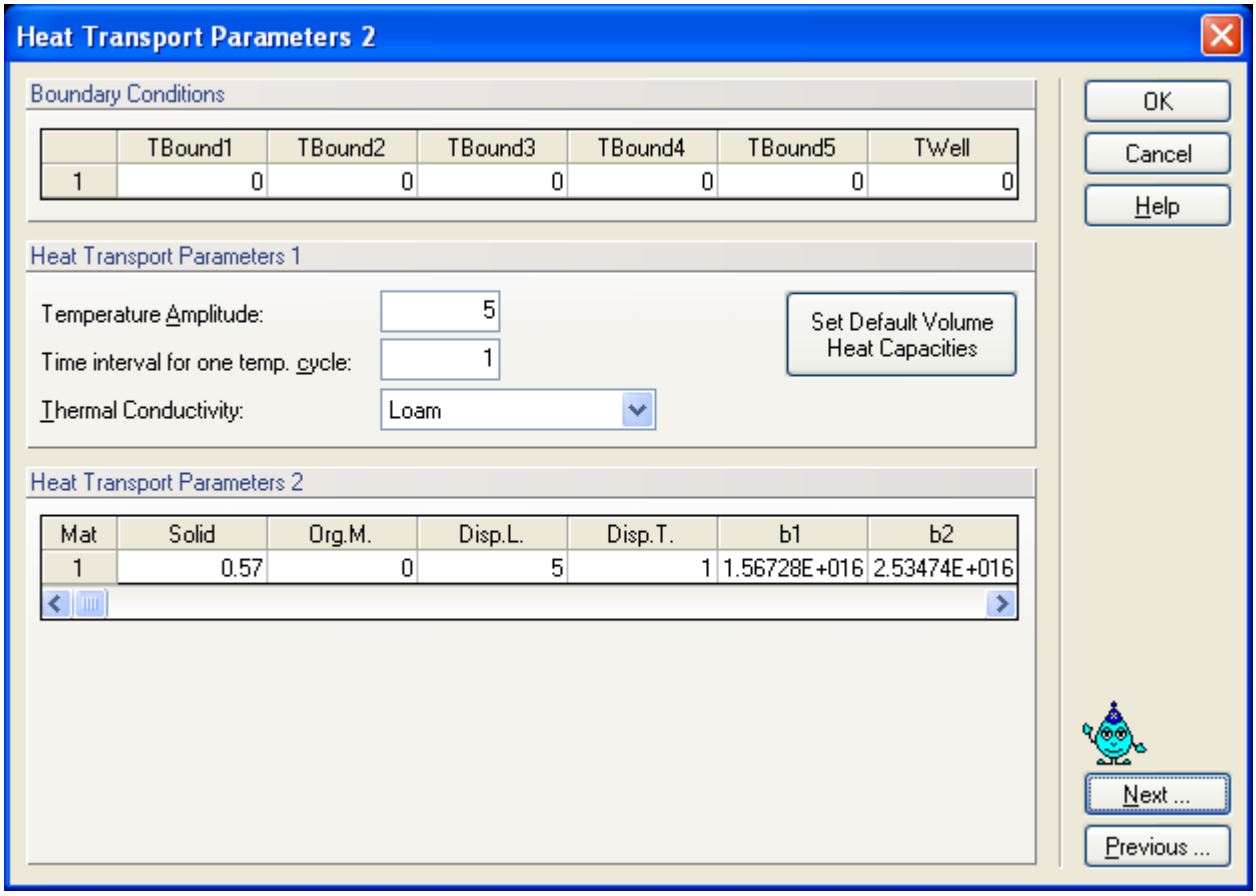


Figure 32. The Heat Transport Parameters dialog window.

The following **Heat Transport Parameters** (bottom part of the dialog window) are specified for each soil material:

Solid Volume fraction of solid phase, θ_n [-]
Org.M. Volume fraction of organic matter, θ_o [-]
Disp.L. Longitudinal thermal dispersivity, λ_L [L]
Disp.T. Longitudinal thermal dispersivity, λ_T [L]
b1 Coefficient b_1 in the expression for the thermal conductivity function [W/L/K]
b2 Coefficient b_2 in the expression for the thermal conductivity function [W/L/K]
b3 Coefficient b_3 in the expression for the thermal conductivity function [W/L/K]
Cn Volumetric heat capacity of the solid phase, C_n [J/L^3/K]
Co Volumetric heat capacity of organic matter, C_o [J/L^3/K]

Cw Volumetric heat capacity of the liquid phase, C_w [J/L^3/K]

Boundary Conditions:
Temperatures for *Boundary Conditions* with time-independent boundary conditions are also specified in this dialog window.

TBound1 Value of the temperature for the first time-independent boundary condition [K]. Set equal to zero if no time-independent boundary condition is specified. The same for TBound2 through TBound4

TWell Value of the temperature for the sixth time-independent boundary condition [K]. If internal sources are specified, then *TWell* is automatically used for the temperature of water injected into the flow region from sources in the transport domain. Set equal to zero if no sixth time-independent boundary condition and no internal sources are specified.

The boundary condition at the soil surface may be approximated using a sinus wave with the maximum one hour after noon and the minimum one hour after midnight as follows:

$$T = T_0 + A\cos\left[2\pi\left(\frac{t-13}{24}\right)\right]$$

where T_0 is the average temperature at the soil surface [K], A is the **Temperature Amplitude** at the soil surface [K], and p is the **Time Interval** for completion of one sine wave temperature (usually 1 day, the default value). The second part of the sine term is included to set the maximum temperature at 1 p.m.

Default values for the parameters in the **Thermal Conductivities** of three textural classes (sand, loam and clay) are provided by HYDRUS [*Chung and Horton*, 1987]. Default volumetric heat capacities for the solid phase, organic matter, and liquid phase are also given (*Set Default Volumetric Heat Capacities*).

When the parameter estimation option is selected, then users must provide initial estimates of the optimized heat transport parameters, specify which parameters are to be optimized (check appropriate checkboxes), and provide parameter constraints for the optimization. Zero values for the minimum and maximum values signify that parameters are unconstrained. The **Heat Transport Parameters** dialog window for the inverse problem is not further shown here.

Notice that thermal conductivity and volumetric heat capacity parameters have units of [$Wm^{-1}K^{-1}$] and [$Jm^{-3}K^{-1}$], respectively. These units, when converted to basic SI units are [$ML^{-1}T^{-2}K^{-1}$] and [$MLT^{-3}K^{-1}$], respectively, and thus contain time to the negative second or third power, which needs to be taken into account during any time conversion.

3.18. *Root Water Uptake Model*

Users may select a particular **Water Uptake Reduction Model** and a **Solute Stress Model** in the **Root Water Uptake Model** dialog window (Fig. 33).

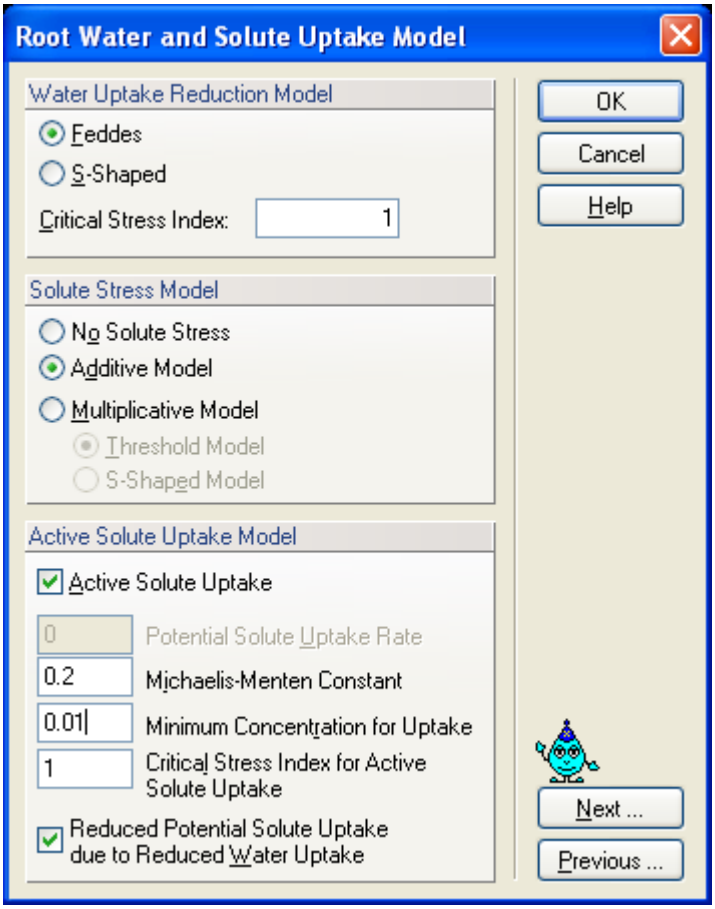


Figure 33. The Root Water Uptake Model dialog window.

a) Water Uptake Reduction Model

Either a water stress response function suggested by *Feddes* et al. [1978] or an S-shaped function suggested by *van Genuchten* [1985] can be used to reduce the potential root water uptake to the actual water uptake rate (Fig. 34). Root water uptake with compensation can be simulated when the *Critical Stress Index* is smaller than one (see the Technical Manual; *Šimůnek et al.* [2010]).

b) Solute Stress Model

The effect of salinity stress on the root water uptake can be either neglected (*No Solute Stress*) or considered using the *Additive* or *Multiplicative* models, i.e., salinity stress is either added to water stress, or uptake reduction due to water stress and salinity stress are multiplied. When the multiplicative model is used for salinity stress, one can use either the *Threshold Model* [*Maas*, 1990] or an *S-Shaped Model* [*van Genuchten*, 1985] (Fig. 35).

c) Active Solute Uptake Model

Total root nutrient uptake is determined from the total of **active** and **passive nutrient uptake.** The partitioning between passive and active uptake is controlled by the a priori defined concentration value **cRoot** (Fig. 26). Passive nutrient uptake is simulated by multiplying root water uptake with the dissolved nutrient concentration, for soil solution concentration values below **cRoot**. Passive nutrient uptake is thus zero when **cRoot** is equal to zero. One must therefore specify the maximum allowed concentration, **cRoot**, in the passive root solute uptake term. When zero is specified, all solute is left behind in the soil (there is no passive root solute uptake) and only solute free solution is taken up. When the concentration is lower than **cRoot**, all solute is taken up (unlimited passive root solute uptake). When the concentration is higher than **cRoot**, additional solute stays behind.

As the **Active Nutrient Uptake** is obtained from the difference between plant nutrient demand (the **Potential Solute Uptake Rate** [$ML^{-2}T^{-1}$] needs to be specified) and **Passive Nutrient Uptake**, the presented model thus implies that reduced passive nutrient uptake is compensated for by active nutrient uptake. Active nutrient uptake is simulated using Michaelis-Menten kinetics (the **Michaelic-Menten constant** and a **Minimum Concentration for Uptake** need to be specified). In addition, the proposed root uptake model includes compensation for active nutrient uptake, in a similar way as used for root water uptake (using the **Critical Stress Index**).

Reduction in root water uptake will decrease passive nutrient uptake, thereby increasing active nutrient uptake proportionally. In other words, total nutrient uptake is not affected by soil water stress, as computed by the proportion of actual to potential root water uptake. This is not realistic since one would expect that plant nutrient requirements will be reduced for water-stressed plants. For that reason, the uptake model includes additional flexibility, by reducing the potential nutrient demand (**Potential Solute Uptake Rate**), in proportion to the reduction of root water uptake (see the last check box **Reduce Potential Solute Uptake due to Reduced Water Uptake**).

Active solute uptake is implemented only for a single solute (not for multiple solutes). Details about the root water and solute uptake can be found in the **Technical Manual** or *Šimůnek and Hopmans* [2009].

3.19. *Root Water Uptake Parameters*

Parameters for the water and salinity stress response functions are specified in the **Root Water Uptake Parameters** dialog window (Fig. 34 and Fig. 35, respectively).

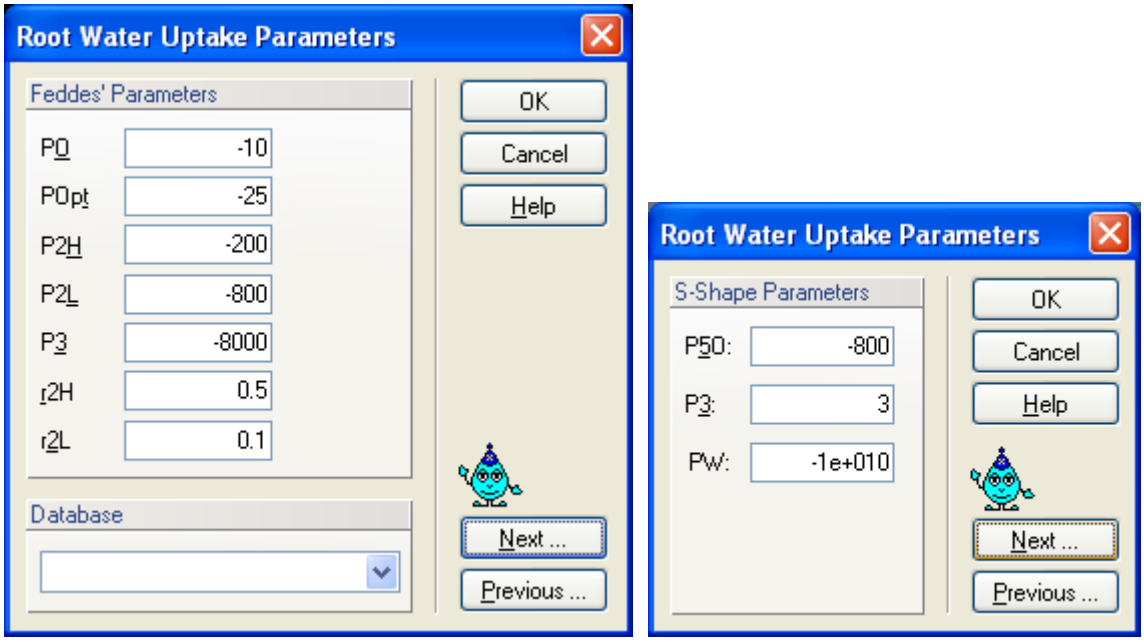


Figure 34. The Root Water Uptake Parameters dialog window for the water stress response function of *Feddes et al.* [1978] (left) and *van Genuchten* [1985] (right).

The **Root Water Uptake Parameters** for the water stress response function suggested by *Feddes et al.* [1978] (Fig. 34, left) are described in detail in the HYDRUS technical manual. Water uptake in this model is assumed to be zero close to saturation (i.e. wetter than some arbitrary "anaerobiosis point" **P0**). Root water uptake is also zero for pressure heads less (more negative) than the wilting point (**P3**). Water uptake is considered optimal between pressure heads **Popt** and **P2**, whereas for pressure heads between **P2** and **P3** (or **P0** and **Popt**) water uptake decreases (or increases) linearly with pressure head.

P0 Value of the pressure head [L] below which roots start to extract water from the soil.

POpt Value of the pressure head [L] below which roots extract water at the maximum possible rate.

P2H Value of the limiting pressure head [L] below which roots cannot longer extract water at the maximum rate (assuming a potential transpiration rate of *r2H*).

P2L As P2H, but for a potential transpiration rate of *r2L*.

P3 Value of the pressure head [L] below which root water uptake ceases (usually taken at the wilting point).

r2H Potential transpiration rate [LT^{-1}] (currently set at 0.5 cm/day).

r2L Potential transpiration rate [LT^{-1}] (currently set at 0.1 cm/day).

The above input parameters permit one to make the variable P2 a function of the potential transpiration rate, T_p (P2 presumably decreases at higher transpiration rates). HYDRUS currently implements the same linear interpolation scheme as used in several versions of the SWATRE code (e.g., *Wesseling and Brandyk*, 1985). The interpolation scheme is defined in the manual.

A database of suggested values for different plants for the *Feddes et al.* [1978] model is provided in HYDRUS based on studies by *Wesseling* [1991] and *Taylor and Ashcroft* [1972].

The **Root Water Uptake Parameters** for the S-shaped water stress response function as suggested by *van Genuchten* [1985] (Fig. 34, right) are as follows:

P50 The coefficient, *h50*, in the root water uptake response function associated with water stress [L]. Root water uptake at this pressure head is reduced by 50%.

P3 The exponent, *p3*, in the root water uptake response function associated with water stress [-]; its recommended and default value is 3.

We have additionally included a parameter **PW**, i.e., pressure head at the wilting point [L], below which transpiration stops.

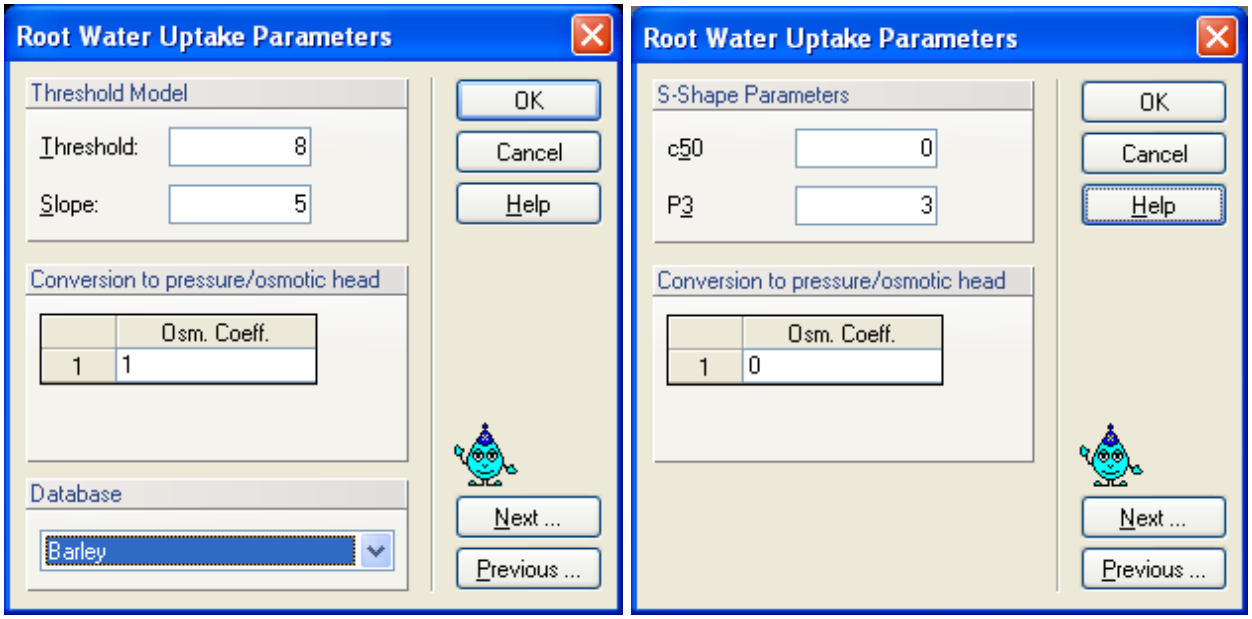


Figure 35. The Root Water Uptake Parameters dialog window for the solute stress response function based on the threshold model (left) and S-shaped model of *van Genuchten* [1985] (right).

The **Root Water Uptake Parameters** for the *Threshold Model* [*Maas*, 1990] of the salinity stress response function (multiplicative) (Fig. 35, left) are as follows:

Threshold Value of the minimum osmotic head [L] (the salinity threshold) above which root water uptake occurs without a reduction.

Slope Slope of the curve determining the fractional root water uptake decline per unit increase in salinity below the threshold.

The **Root Water Uptake Parameters** for the *S-Shaped Model* [*van Genuchten*, 1985] of the salinity stress response function (multiplicative) (Fig. 35, right) are as follows:

P3 The exponent, *p*, in the root water uptake response function associated with salinity stress [-]. The recommended value is 3.

c50 The coefficient, *h50*, in the root water uptake response function associated with salinity stress [L]. Root water uptake at this osmotic head is reduced by 50%.

Both salinity stress response functions require a coefficient (*Osmotic Coefficient*) that transforms concentrations into equivalent osmotic pressure heads (Fig. 35). The osmotic coefficients should be negative for the additive model (to be added to negative pressure heads) and positive for the multiplicative model. Note that this conversion needs to be made mainly when one uses the **Additive Model**. That is because then one needs to **add** pressure heads (i.e., units of m or cm) and osmotic heads (calculated from concentrations, which likely have units of dS/m). If one uses the **Multiplicative Model** then one does not need to use this conversion, and can keep **Osm. Coeff** equal to one, since a) both water stress and salinity stress response functions can have their own units, and b) both the **Threshold Model** parameters (specified above) and selected concentrations units are likely already the same (e.g., units of EC (dS/m)).

A database of suggested values for different plants for the threshold-slope salinity stress model is provided based on the work by *Maas* [1990]. The database for the threshold model provides suggested values based on the electric conductivity of the saturation extract EC_e in dS/m. These values are converted internally in the GUI into the electric conductivity of soil water (at the field capacity) as follows: $EC_w \approx k_e * EC_e$, where k_e is approximately 2 [*Skaggs et al.*, 2006]. Consequently, the threshold value of Maas [1990] is multiplied by 2 (k_e) and the slope is divided by 2. A user is responsible for converting these values in the regular HYDRUS further to the osmotic pressure in the head units [L] or concentration units used in your project. For guidance, see Eqs. 13.3 and 13.4 in *Maas* [1990].

The threshold-slope salinity stress model is implemented in the standard HYDRUS solute transport model as $R = 1 - 0.01(c - c_T)s$, while in the UNSATCHEM module as $R = 1 + (h_\phi - h_{\phi T})s^*$, where c_T is the concentration threshold, $h_{\phi T}$ is the osmotic head threshold, s is the slope in HYDRUS and s^* is the slope in UNSATCHEM.

3.20. *Root Distribution Parameters*

The spatial distribution of the roots can be specified using the **Root Distribution Parameters** dialog window (Fig. 36). The following two- and three-dimensional root distribution functions are implemented in HYDRUS [*Vrugt et al.*, 2001, 2002]:

$$b(x,z)=\left(1-\frac{z}{Z_m}\right)\left(1-\frac{x}{X_m}\right)e^{-\left(\frac{p_z}{Z_m}\left|z^*-z\right|+\frac{p_r}{X_m}\left|x^*-x\right|\right)}$$

$$b(x,y,z)=\left(1-\frac{x}{X_m}\right)\left(1-\frac{y}{Y_m}\right)\left(1-\frac{z}{Z_m}\right)e^{-\left(\frac{p_x}{X_m}\left|x^*-x\right|+\frac{p_y}{Y_m}\left|y^*-y\right|+\frac{p_z}{Z_m}\left|z^*-z\right|\right)}$$

where X_m, Y_m, and Z_m are the maximum rooting lengths in the *x*-, *y*-, and *z*- directions [L], respectively; *x*, *y*, and *z* are distances from the origin of the plant (tree) in the *x*-, *y*-, and *z*-directions [L], respectively; p_x [-], p_y [-], p_z [-], x^* [L], y^* [L], and z^* [L] are empirical parameters (x^*, y^*, and z^* are in Fig. 36 indicated as *Depth of Maximum Intensity* or *Radius of Maximum Intensity*; parameters p_x, p_y, and p_z are assumed to be zero for $x> x^*$, $y> y^*$, $z> z^*$, respectively [*Vrugt et al.*, 2002]), and $b(x,z)$ and $b(x,y,z)$ denote two- and three-dimensional spatial distribution of the potential root water uptake [-]. See *Vrugt et al*. [2001, 2002] for different configurations of the normalized spatial distribution of potential root water uptake rate. The equations above are given and used in absolute coordinates, i.e., they are independent of any actual selection in GUI. The *x* and *y* coordinates are identical to *x* and *y* coordinates for the geometry of the transport domain. The only exception is that the beginning of the *z* coordinate for the root distribution starts at the highest located node of the entire transport domain (again independent of any actual selection).

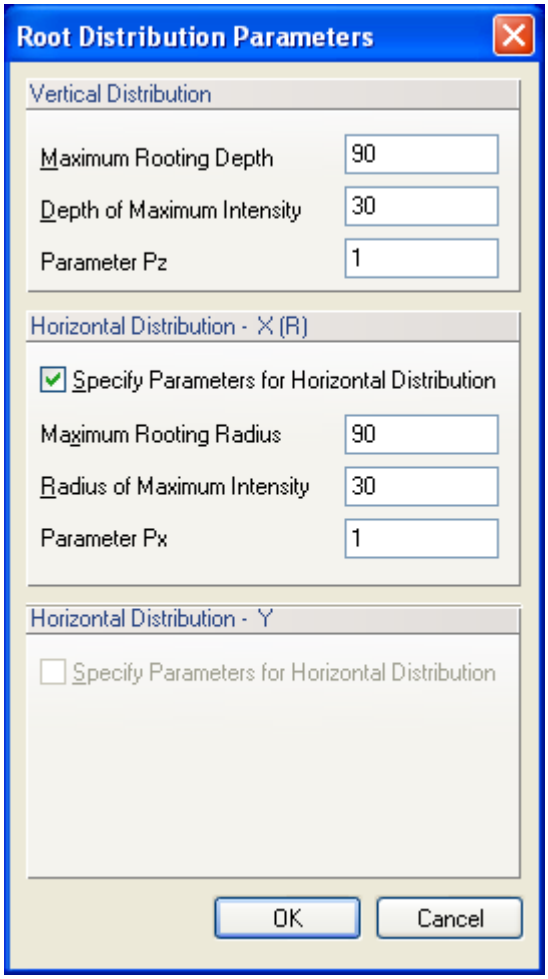
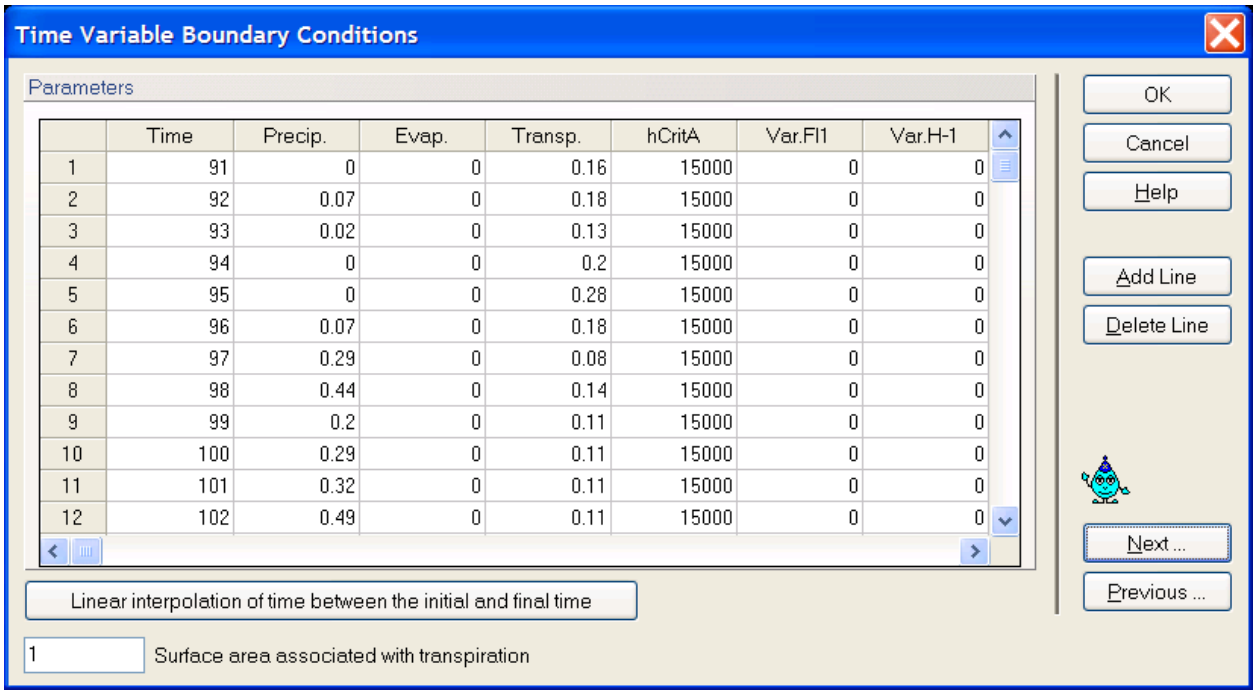


Figure 36. The Root Distribution Parameters dialog window.

3.21. *Time Variable Boundary Conditions*

The **Time Variable Boundary Conditions** dialog window is shown in Figure 37.



	Time	Precip.	Evap.	Transp.	hCritA	Var.Fl1	Var.H-1
1	91	0	0	0.16	15000	0	0
2	92	0.07	0	0.18	15000	0	0
3	93	0.02	0	0.13	15000	0	0
4	94	0	0	0.2	15000	0	0
5	95	0	0	0.28	15000	0	0
6	96	0.07	0	0.18	15000	0	0
7	97	0.29	0	0.08	15000	0	0
8	98	0.44	0	0.14	15000	0	0
9	99	0.2	0	0.11	15000	0	0
10	100	0.29	0	0.11	15000	0	0
11	101	0.32	0	0.11	15000	0	0
12	102	0.49	0	0.11	15000	0	0

Figure 37. The Time Variable Boundary Conditions dialog window.

The following variables are specified in the **Time Variable Boundary Conditions** dialog window:

Time Time for which a data record is provided [T].

Precip Precipitation rate [LT^{-1}] (in absolute value) (applied to the atmospheric boundary).

Evap Potential evaporation rate [LT^{-1}] (in absolute value) (applied to the atmospheric boundary).

Trans Potential transpiration rate [LT^{-1}] (in absolute value).

hCritA Absolute value of the minimum allowed pressure head at the soil surface [L] (applied to the atmospheric boundary).

Var.Fl1 Drainage flux [LT^{-1}] across the bottom boundary, or another time-dependent prescribed flux boundary condition (positive when water leaves the flow region); set to zero when no time-dependent flux boundary condition is specified. Same for Var.Fl2, Var.Fl3, or Var.Fl4. The Var.Fl4 value is used for internal time-variable nodal flux sinks or sources (if they exist).

Var.H-1 Groundwater level [L] (usually negative), or other time-dependent prescribed head boundary condition; set equal to zero when no time-dependent head boundary

condition is specified. Same for Var.H-2, Var.H-3, or Var.H-4. The Var. H-4 value is used for internal time-variable nodal pressure head sinks or sources (if they exist).

TVal1 The first time-dependent temperature [K] that can be used for nodes with time variable boundary conditions (atmospheric BC, variable head/flux BC) (is not specified when heat transport or time variable boundary conditions are not considered).

TVal2 The second time-dependent temperature [K] that can be used for nodes with time variable boundary conditions (is not specified when heat transport or time variable boundary conditions are not considered).

CVal1 The first time-dependent solute concentration [ML^{-3}] that can be used for nodes with prescribed time variable boundary conditions (atmospheric BC, variable head/flux BC) (not specified when solute transport is not considered). This column should be used preferably only for the atmospheric boundary, because the concentration value is adjusted based on values of precipitation and evaporation as follows: cVal1=Precip/(Precip-Evap)*cVal1. The cVal1 is adjusted to be zero when Evap > Precip. Similar adjustments are not done for cVal2, and other concentration values.

CVal2 The second time-dependent solute concentration [ML^{-3}] that can be used for nodes with prescribed time variable boundary conditions (atmospheric BC, variable head/flux BC) (not specified when solute transport is not considered).

CVal3 The third time-dependent solute concentration [ML^{-3}] that can be used for nodes with prescribed time variable boundary conditions (atmospheric BC, variable head/flux BC) (not specified when solute transport is not considered).

The last three entries are entered for each solute.

The table in Figure 37 can be edited by manually adding or deleting lines. The table has a capacity for about 32,000 records (depends on the number of columns). When a longer time record is to be simulated, then one needs to directly edit the Atmosph.in input file in the working directory using any standard software, such as MS Excel. The manually modified Atmosph.in file then needs to be imported back into the HYDRUS *project_name.h32d* file using the command *File->Import and Export->Import Input Data from *.In Files*. Data for the **Time Variable Boundary Conditions** can be prepared in any spreadsheet software and then copied into the table using Windows paste hot keys (i.e., Ctrl+V).

The total number of atmospheric data records is given in the Main Time Information dialog window (Fig. 15).

3.22. *Constructed Wetlands*

Two biokinetic model formulations can be chosen: (1) the biokinetic model as described in CW2D [*Langergraber and Šimůnek*, 2005, 2006] and (2) the CWM1 (Constructed Wetland Model #1) biokinetic model [*Langergraber et al.*, 2009]. In CW2D aerobic and anoxic transformation and degradation processes for organic matter, nitrogen and phosphorus are described, whereas in CWM1 aerobic, anoxic and anaerobic processes for organic matter, nitrogen and sulphur. Comparisons between CW2D and CWM1 components and processes is given in Tables 11 and 12, respectively. Details about both modules can be found in the above referenced literature.

Parameters for constructed wetlands are entered in the **Constructed Wetland Model Parameters I and II** dialog windows for the CW2D (Fig. 38 and 40, respectively) and CWM1 (Fig. 39 and 41, respectively) modules.

Table 11. Comparison of CW2D and CWM1 components.

CW2D	**CWM1**
[*Langergraber and Šimunek*, 2005]	[*Langergraber et al.*, 2009]
Components 1. **SO**: *Dissolved oxygen*, O2. 2. **CR**: *Readily biodegradable soluble COD*. 3. **CS**: *Slowly biodegradable soluble COD*. 4. **CI**: *Inert soluble COD*. 5. **XH**: *Heterotrophic bacteria* 6. **XANs**: *Autotrophic ammonia oxidizing bacteria (Nitrosomonas spp.)* 7. **XANb**: *Autotrophic nitrite oxidizing bacteria (Nitrobacter spp.)* 8. **NH4N:** *Ammonium and ammonia nitrogen*. 9. **NO2N:** *Nitrite nitrogen*. 10. **NO3N:** *Nitrate nitrogen*. 11. **N2:** *Elemental nitrogen.* 12. **PO4P:** Phosphate phosphorus Organic nitrogen and organic phosphorus are modeled as part of the COD. Nitrification is modeled as to-step process. Bacteria are assumed to be immobile.	**Soluble components, S?** 1. **SO**: *Dissolved oxygen*, O2. 2. **SF**: *Fermentable, readily biodegradable soluble COD*. 3. **SA**: *Fermentation products as acetate*. 4. **SI**: *Inert soluble COD*. 5. **SNH**: *Ammonium and ammonia nitrogen*. 6. **SNO**: *Nitrate and nitrite nitrogen*. 7. **SSO4**: *Sulphate sulphur*. 8. **SH2S**: *Dihydrogensulphide sulphur*. **Particulate components, X?** 9. **XS**: *Slowly biodegradable particulate COD*. 10. **XI**: *Inert particulate COD*. 11. **XH**: *Heterotrophic bacteria*. 12. **XA**: *Autotrophic nitrifying bacteria*. 13. **XFB**: *Fermenting bacteria*. 14. **XAMB**: *Acetotrophic methanogenic bacteria*. 15. **XASRB**: *Acetotrophic sulphate reducing bacteria*. 16. **XSOB**: *Sulphide oxidizing bacteria*. Organic nitrogen and organic phosphorus are modeled as part of the COD.

Table 12. Comparison of CW2D and CWM1 processes.

CW2D	**CWM1**
[*Langergraber and Šimunek*, 2005]	[*Langergraber et al.*, 2009]
Heterotrophic bacteria: 1. ***Hydrolysis***: conversion of CS into CR. 2. ***Aerobic growth of XH on CR*** (mineralization of organic matter). 3. ***Anoxic growth of XH on CR*** (denitrification on NO2N). 4. ***Anoxic growth of XH on CR*** (denitrification on NO3N). 5. ***Lysis of XH***. ***Autotrophic bacteria:*** 6. ***Aerobic growth of XANs on SNH*** (ammonium oxidation). 7. ***Lysis of XANs***. 8. ***Aerobic growth of XANb on SNH*** (nitrite oxidation). 9. ***Lysis of XANb***.	***Heterotrophic bacteria:*** 1. ***Hydrolysis***: conversion of XS into SF. 2. ***Aerobic growth of XH on SF*** (mineralization of organic matter). 3. ***Aerobic growth of XH on SA*** (mineralization of organic matter). 4. ***Anoxic growth of XH on SF*** (denitrification). 5. ***Anoxic growth of XH on SA*** (denitrification). 6. ***Lysis of XH***. ***Autotrophic bacteria:*** 7. ***Aerobic growth of XA on SNH*** (nitrification). 8. ***Lysis of XA***. ***Fermenting bacteria:*** 9. ***Growth of XFB*** (fermentation). 10. ***Lysis of XFB***. ***Acetotrophic methanogenic bacteria:*** 11. ***Growth of XAMB***: Anaerobic growth of acetotrophic, methanogenic bacteria XAMB on acetate SA. 12. ***Lysis of XAMB***. ***Acetotrophic sulphate reducing bacteria:*** 13. ***Growth of XASRB***: Anaerobic growth of acetotrophic, sulphate reducing bacteria. 14. ***Lysis of XASRB***. ***Sulphide oxidizing bacteria:*** 15. ***Aerobic growth of XSOB on SH2S***: The opposite process to process 13, the oxidation of SH2S to SSO4. 16. ***Anoxic growth of XSOB on SH2S***: Similar to process 15 but under anoxic conditions. 17. ***Lysis of XSOB***.

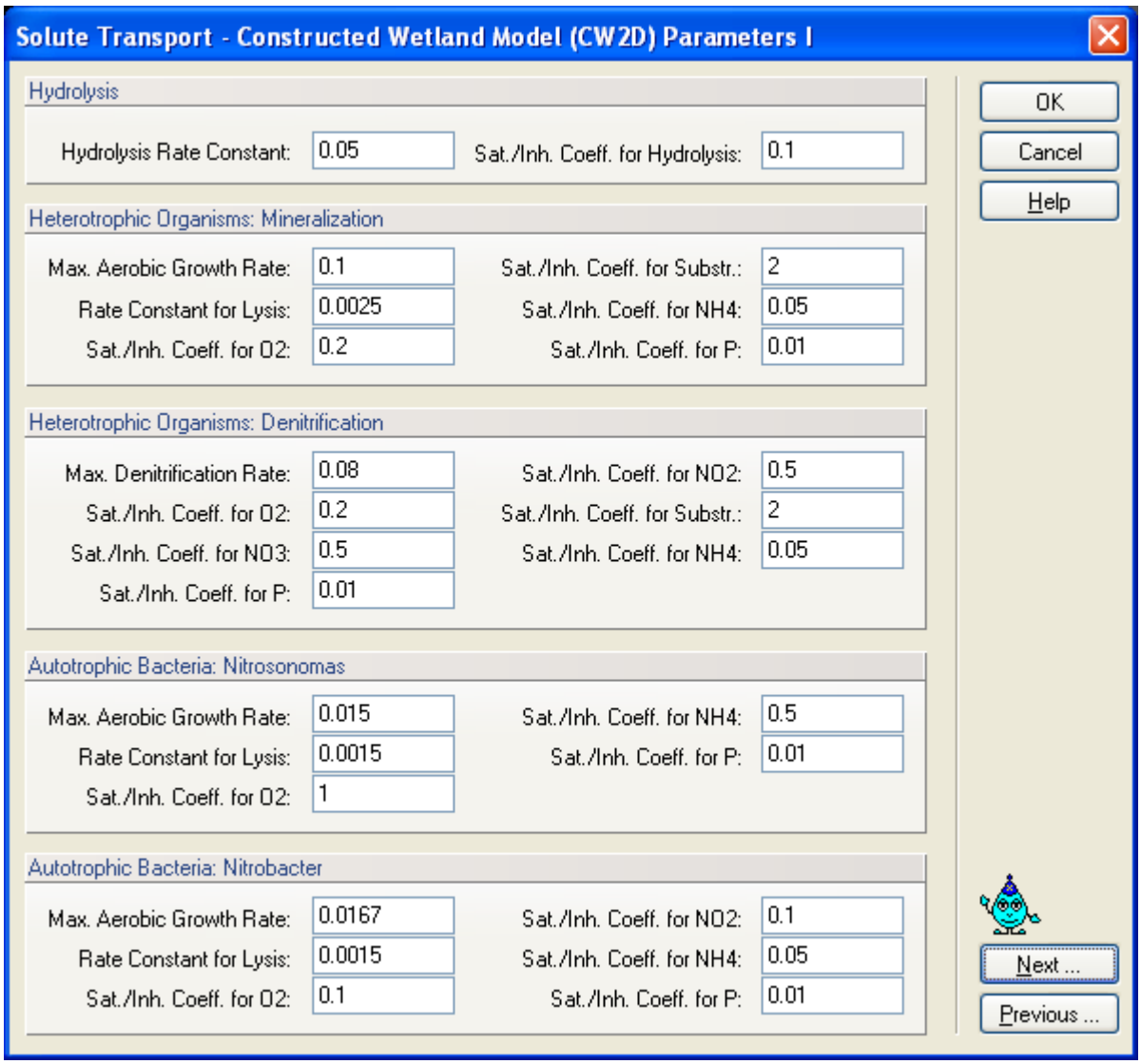

Solute Transport - Constructed Wetland Model (CW2D) Parameters I
Hydrolysis
Hydrolysis Rate Constant: 0.05
Sat./Inh. Coeff. for Hydrolysis: 0.1
Heterotrophic Organisms: Mineralization
Max. Aerobic Growth Rate: 0.1
Rate Constant for Lysis: 0.0025
Sat./Inh. Coeff. for O2: 0.2
Sat./Inh. Coeff. for Substr.: 2
Sat./Inh. Coeff. for NH4: 0.05
Sat./Inh. Coeff. for P: 0.01
Heterotrophic Organisms: Denitrification
Max. Denitrification Rate: 0.08
Sat./Inh. Coeff. for O2: 0.2
Sat./Inh. Coeff. for NO3: 0.5
Sat./Inh. Coeff. for P: 0.01
Sat./Inh. Coeff. for NO2: 0.5
Sat./Inh. Coeff. for Substr.: 2
Sat./Inh. Coeff. for NH4: 0.05
Autotrophic Bacteria: Nitrosonomas
Max. Aerobic Growth Rate: 0.015
Rate Constant for Lysis: 0.0015
Sat./Inh. Coeff. for O2: 1
Sat./Inh. Coeff. for NH4: 0.5
Sat./Inh. Coeff. for P: 0.01
Autotrophic Bacteria: Nitrobacter
Max. Aerobic Growth Rate: 0.0167
Rate Constant for Lysis: 0.0015
Sat./Inh. Coeff. for O2: 0.1
Sat./Inh. Coeff. for NO2: 0.1
Sat./Inh. Coeff. for NH4: 0.05
Sat./Inh. Coeff. for P: 0.01
OK
Cancel
Help
Next ...
Previous ...

Figure 38. The Constructed Wetland Model (CW2D) Parameter I dialog window.

Table 13. Kinetic parameters in the CW2D biokinetic model [*Langergraber and Šimůnek*, 2005].

	Description [unit]	**Value**
Hydrolysis		for 20°C (10°C)
K_h	hydrolysis rate constant [1/d]	3 (2)
K_X	saturation/inhibition coefficient for hydrolysis [g COD_{CS}/g COD_{BM}]	0.1 (0.22)
Heterotrophic bacteria (aerobic growth)		
μ_H	maximum aerobic growth rate on CR [1/d]	6 (3)
b_H	rate constant for lysis [1/d]	0.4 (0.2)
$K_{het,O2}$	saturation/inhibition coefficient for S_O [mg O_2/L]	0.2
$K_{het,CR}$	saturation/inhibition coefficient for substrate [mg COD_{CR}/L]	2
$K_{het,NH4N}$	saturation/inhibition coefficient for NH4 (nutrient) [mg N/L]	0.05
$K_{het,IP}$	saturation/inhibition coefficient for P [mg N/L]	0.01
Heterotrophic bacteria (denitrification)		
μ_{DN}	maximum aerobic growth rate on CR [1/d]	4.8 (2.4)
$K_{het,O2}$	saturation/inhibition coefficient for S_O [mg O_2/L]	0.2
$K_{het,NO3N}$	saturation/inhibition coefficient for NO3 [mg N/L]	0.5
$K_{het,NO2N}$	saturation/inhibition coefficient for NO2 [mg N/L]	0.5
$K_{het,CR}$	saturation/inhibition coefficient for substrate [mg COD_{CR}/L]	4
$K_{het,NH4N}$	saturation/inhibition coefficient for NH4 (nutrient) [mg N/L]	0.05
$K_{het,IP}$	saturation/inhibition coefficient for P [mg N/L]	0.01
Ammonia oxidising bacteria (*Nitrosomonas* spp.)		
μ_{ANs}	maximum aerobic growth rate on S_{NH} [1/d]	0.9 (0.3)
b_{ANs}	rate constant for lysis [1/d]	0.15 (0.05)
$K_{ANs,O2}$	saturation/inhibition coefficient for S_O [mg O_2/L]	1
$K_{ANs,NH4N}$	saturation/inhibition coefficient for NH4 [mg N/L]	0.5
$K_{ANs,IP}$	saturation/inhibition coefficient for P [mg N/L]	0.01
Nitrite oxidising bacteria (*Nitrobacter* spp.)		
μ_{ANb}	maximum aerobic growth rate on S_{NH} [1/d]	1 (0.35)
b_{ANb}	rate constant for lysis [1/d]	0.15 (0.05)
$K_{ANb,O2}$	saturation/inhibition coefficient for S_O [mg O_2/L]	0.1
$K_{ANb,NO2N}$	saturation/inhibition coefficient for NO2 [mg N/L]	0.1
$K_{ANb,NH4N}$	saturation/inhibition coefficient for NH4 (nutrient) [mg N/L]	0.05
$K_{ANb,IP}$	saturation/inhibition coefficient for P [mg N/L]	0.01

Table 14. Kinetic parameters in the CWM1 biokinetic model [*Langergraber et al.*, 2009].

Parameter	Description [unit]	Value
Hydrolysis		for 20°C (10°C)
K_h	hydrolysis rate constant [1/d]	3 (2)
K_X	saturation/inhibition coefficient for hydrolysis [g COD_{SF}/g COD_{BM}]	0.1 (0.22)
η_H	correction factor for hydrolysis by fermenting bacteria [-]	0.1
Heterotrophic bacteria (aerobic growth and denitrification)		
μ_H	maximum aerobic growth rate on S_F and S_A [1/d]	6 (3)
η_g	correction factor for denitrification by XH [-]	0.8
b_H	rate constant for lysis [1/d]	0.4 (0.2)
K_{OH}	saturation/inhibition coefficient for S_O [mg O_2/L]	0.2
K_{SF}	saturation/inhibition coefficient for S_F [mg COD_{SF}/L]	2
K_{SA}	saturation/inhibition coefficient for S_A [mg COD_{SA}/L]	4
K_{NOH}	saturation/inhibition coefficient for S_{NO} [mg N/L]	0.5
K_{NHH}	saturation/inhibition coefficient for S_{NH} (nutrient) [mg N/L]	0.05
K_{H2SH}	saturation/inhibition coefficient for S_{H2S} [mg S/L]	140
Autotrophic bacteria		
μ_A	maximum aerobic growth rate on S_{NH} [1/d]	1 (0.35)
b_A	rate constant for lysis [1/d]	0.15 (0.05)
K_{OA}	saturation/inhibition coefficient for S_O [mg O_2/L]	1
K_{NHA}	saturation/inhibition coefficient for S_{NH} [mg N/L]	0.5 (5)
K_{H2SA}	saturation/inhibition coefficient for S_{H2S} [mg S/L]	140
Fermenting bacteria		
μ_{FB}	maximum aerobic growth rate for X_{FB} [1/d]	3 (1.5)
b_{FB}	rate constant for lysis [1/d]	0.02
K_{OFB}	saturation/inhibition coefficient for S_O [mg O_2/L]	0.2
K_{SFB}	saturation/inhibition coefficient for S_F [mg COD_{SF}/L]	28
K_{NOFB}	saturation/inhibition coefficient for S_{NO} [mg N/L]	0.5
K_{NHFB}	saturation/inhibition coefficient for S_{NH} (nutrient) [mg N/L]	0.01
K_{H2SFB}	saturation/inhibition coefficient for S_{H2S} [mg S/L]	140
Acetotrophic methanogenic bacteria		
μ_{AMB}	maximum aerobic growth rate on for X_{AMB} [1/d]	0.085
b_{AMB}	rate constant for lysis [1/d]	0.008
K_{OAMB}	saturation/inhibition coefficient for S_O [mg O_2/L]	0.0002
K_{SAMB}	saturation/inhibition coefficient for S_A [mg COD_{SA}/L]	56
K_{NOAMB}	saturation/inhibition coefficient for S_{NO} [mg N/L]	0.0005
K_{NHAMB}	saturation/inhibition coefficient for S_{NH} (nutrient) [mg N/L]	0.01
K_{H2SAMB}	saturation/inhibition coefficient for S_{H2S} [mg S/L]	140
Acetotrophic sulphate reducing bacteria		
μ_{ASRB}	maximum aerobic growth rate for X_{ASRB} [1/d]	0.18
b_{ASRB}	rate constant for lysis [1/d]	0.012
K_{OASRB}	saturation/inhibition coefficient for S_O [mg O_2/L]	0.0002
K_{SASRB}	saturation/inhibition coefficient for S_A [mg COD_{SA}/L]	24
K_{NOASRB}	saturation/inhibition coefficient for S_{NO} [mg N/L]	0.0005
K_{NHASRB}	saturation/inhibition coefficient for S_{NH} (nutrient) [mg N/L]	0.01
K_{SOASRB}	saturation/inhibition coefficient for S_{SO4} [mg S/L]	19
$K_{H2SASRB}$	saturation/inhibition coefficient for S_{H2S} [mg S/L]	140

Sulphide oxidising bacteria		
μ_{SOB}	maximum aerobic growth rate for X_{SOB} [1/d]	5.28
η_{SOB}	correction factor for anoxic growth of X_{SOB} [-]	0.8
b_{SOB}	rate constant for lysis [1/d]	0.15
K_{OSOB}	saturation/inhibition coefficient for S_O [mg O_2/L]	0.2
K_{NOSOB}	saturation/inhibition coefficient for S_{NO} [mg N/L]	0.5
K_{NHSOB}	saturation/inhibition coefficient for S_{NH} (nutrient) [mg N/L]	0.05
K_{SSOB}	saturation/inhibition coefficient for S_{H2S} [mg S/L]	0.24

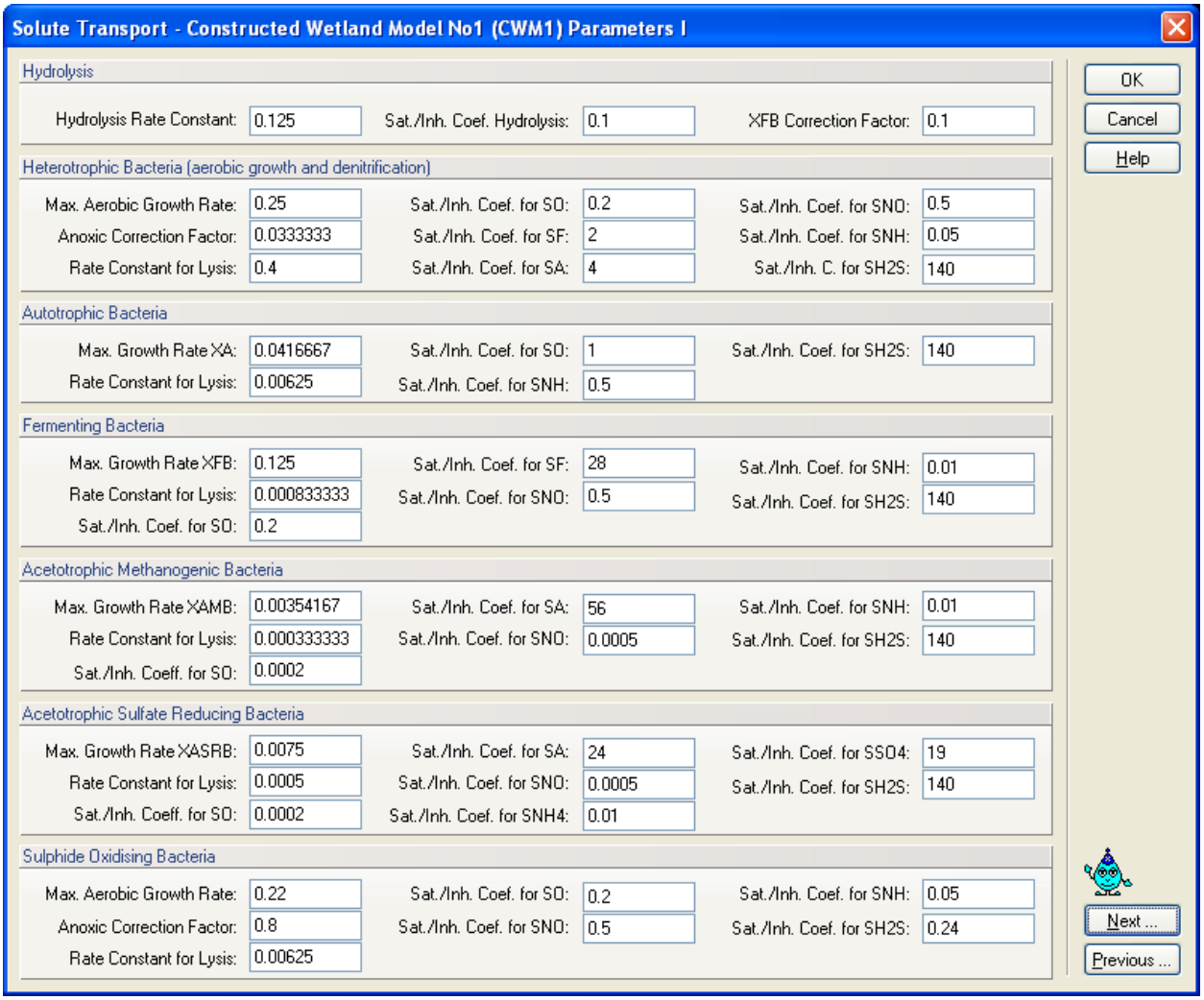

Solute Transport - Constructed Wetland Model No1 (CWM1) Parameters I
Hydrolysis
Hydrolysis Rate Constant: 0.125
Sat./Inh. Coef. Hydrolysis: 0.1
XFB Correction Factor: 0.1
Heterotrophic Bacteria (aerobic growth and denitrification)
Max. Aerobic Growth Rate: 0.25
Anoxic Correction Factor: 0.0333333
Rate Constant for Lysis: 0.4
Sat./Inh. Coef. for SO: 0.2
Sat./Inh. Coef. for SF: 2
Sat./Inh. Coef. for SA: 4
Sat./Inh. Coef. for SNO: 0.5
Sat./Inh. Coef. for SNH: 0.05
Sat./Inh. C. for SH2S: 140
Autotrophic Bacteria
Max. Growth Rate XA: 0.0416667
Rate Constant for Lysis: 0.00625
Sat./Inh. Coef. for SO: 1
Sat./Inh. Coef. for SNH: 0.5
Sat./Inh. Coef. for SH2S: 140
Fermenting Bacteria
Max. Growth Rate XFB: 0.125
Rate Constant for Lysis: 0.000833333
Sat./Inh. Coef. for SO: 0.2
Sat./Inh. Coef. for SF: 28
Sat./Inh. Coef. for SNO: 0.5
Sat./Inh. Coef. for SNH: 0.01
Sat./Inh. Coef. for SH2S: 140
Acetotrophic Methanogenic Bacteria
Max. Growth Rate XAMB: 0.00354167
Rate Constant for Lysis: 0.000333333
Sat./Inh. Coeff. for SO: 0.0002
Sat./Inh. Coef. for SA: 56
Sat./Inh. Coef. for SNO: 0.0005
Sat./Inh. Coef. for SNH: 0.01
Sat./Inh. Coef. for SH2S: 140
Acetotrophic Sulfate Reducing Bacteria
Max. Growth Rate XASRB: 0.0075
Rate Constant for Lysis: 0.0005
Sat./Inh. Coeff. for SO: 0.0002
Sat./Inh. Coef. for SA: 24
Sat./Inh. Coef. for SNO: 0.0005
Sat./Inh. Coef. for SNH4: 0.01
Sat./Inh. Coef. for SSO4: 19
Sat./Inh. Coef. for SH2S: 140
Sulphide Oxidising Bacteria
Max. Aerobic Growth Rate: 0.22
Anoxic Correction Factor: 0.8
Rate Constant for Lysis: 0.00625
Sat./Inh. Coef. for SO: 0.2
Sat./Inh. Coef. for SNO: 0.5
Sat./Inh. Coef. for SNH: 0.05
Sat./Inh. Coef. for SH2S: 0.24
OK
Cancel
Help
Next ...
Previous ...

Figure 39. The Constructed Wetland Model (CWM1) Parameter I dialog window.

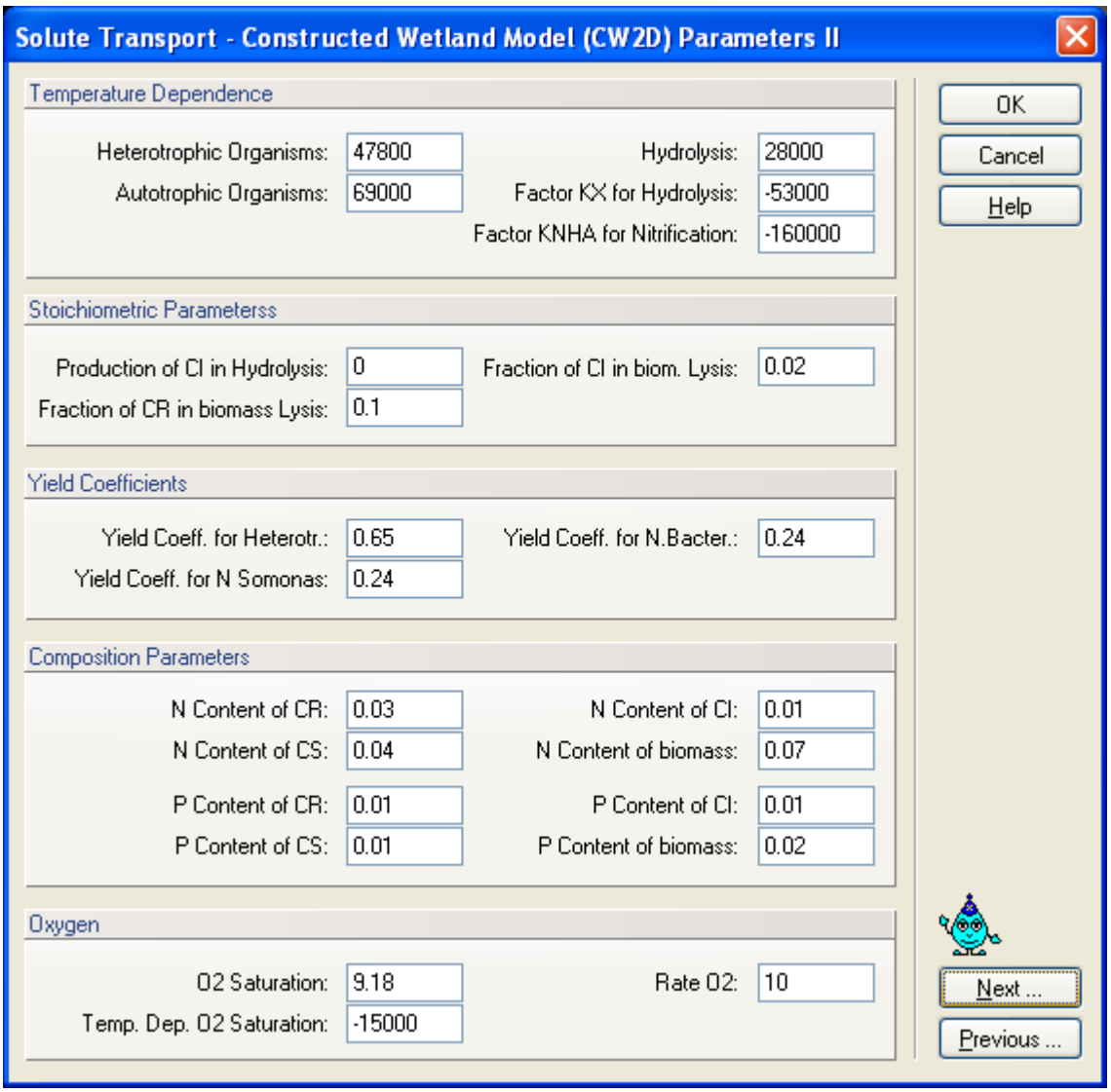


Figure 40. The Constructed Wetland Model (CW2D) Parameter II dialog window.

Table 15. Temperature dependences, stoichiometric parameters, composition parameters and parameters describing oxygen transfer in the CW2D biokinetic model [*Langergraber and Šimunek*, 2005].

Parameter	Description [unit]	Value
Temperature dependences (activation energy [J/mol] for Arrhenius equation**)**		
Tdep_het	activation energy for processes caused by XH [J/mol]	47800
Tdep_aut	activation energy for processes caused by XA [J/mol]	69000
Tdep_Kh	activation energy Hydrolyses [J/mol]	28000
Tdep_KX	activation energy factor KX for hydrolyses [J/mol]	-53000
Tdep_KNHA	activation energy for factor KNHA for nitrification [J/mol]	-160000
Stoichiometric parameters		
$f_{Hyd,CI}$	production of CI in hydrolysis	0.0
$f_{BM,CR}$	fraction of CR generated in biomass lysis	0.1
$f_{BM,CI}$	fraction of CI generated in biomass lysis	0.02
Y_{Het}	yield coefficient for XH	0.63
Y_{ANs}	yield coefficient for XANs	0.24
Y_{ANb}	yield coefficient for XANb	0.24
Composition parameters		
$i_{N,CR}$	N content of CR [g N/g COD_{CR}]	0.03
$i_{N,CS}$	N content of CS [g N/g COD_{CS}]	0.04
$i_{N,CI}$	N content of CI [g N/g COD_{CI}]	0.01
$i_{N,BM}$	N content of biomass [g N/g COD_{BM}]	0.07
$i_{P,CR}$	P content of CR [g P/g COD_{CR}]	0.01
$i_{P,CS}$	P content of CS [g P/g COD_{CS}]	0.01
$i_{P,CI}$	P content of CI [g P/g COD_{CI}]	0.01
$i_{P,BM}$	P content of biomass [g P/g COD_{BM}]	0.02
Oxygen		
cO2_sat_20	saturation concentration of oxygen [g/m³]	9.18
Tdep_cO2_sat	activation energy for saturation concentration of oxygen [J/mol]	-15000
rate_O2	re-aeration rate [1/d]	240

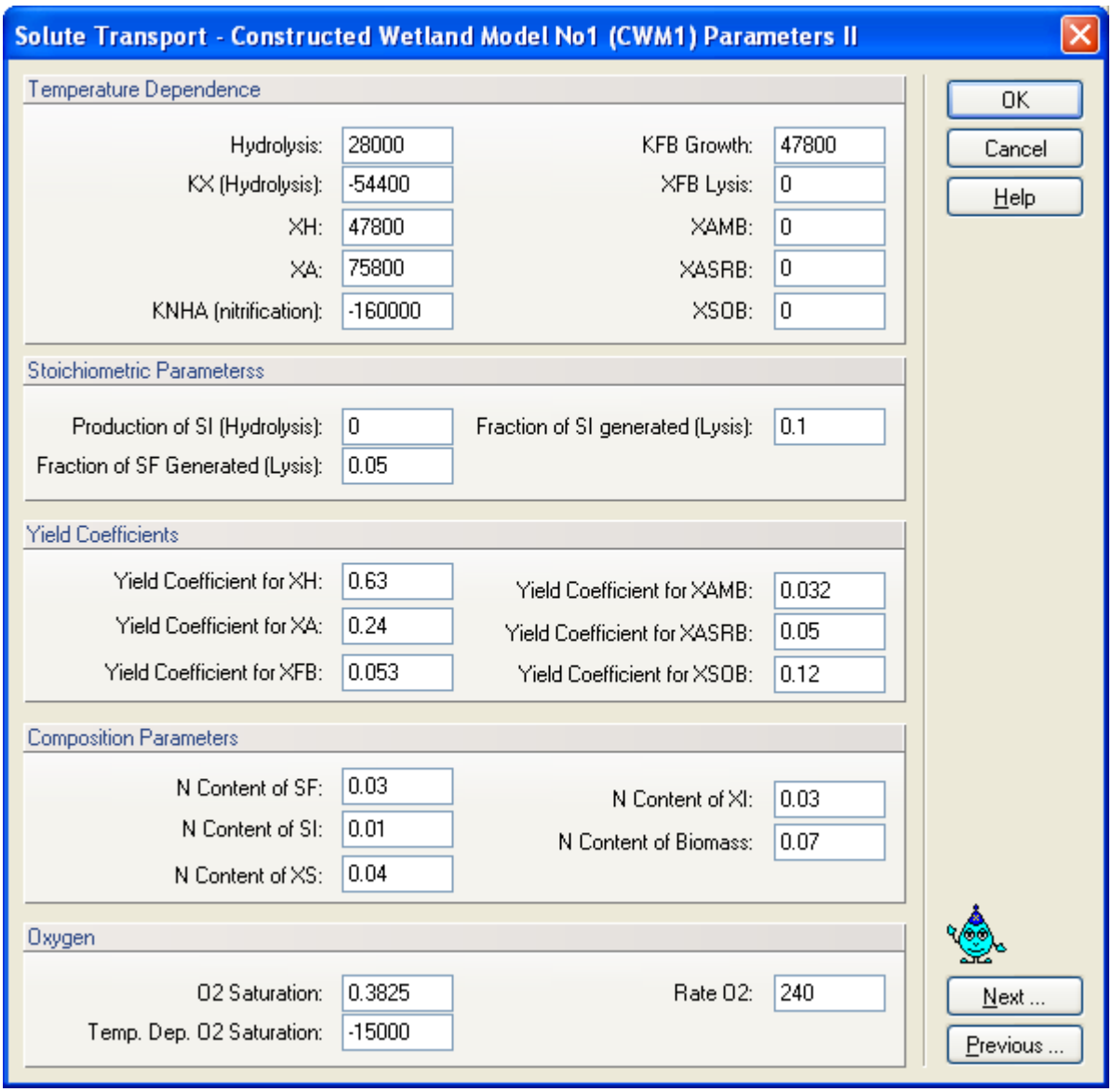


Figure 41. The Constructed Wetland Model (CWM1) Parameter II dialog window.

Table 16. Temperature dependences, stoichiometric parameters, composition parameters and parameters describing oxygen transfer in the CWM1 biokinetic model [*Langergraber et al.*, 2009].

Parameter	Description [unit]	Value
Temperature dependences (activation energy [J/mol] for Arrhenius equation**)**		
Tdep_HyKh	activation energy Hydrolyses [J/mol]	28000
Tdep_HyKX	activation energy factor KX for hydrolyses [J/mol]	-54400
Tdep_H	activation energy for processes caused by XH [J/mol]	47800
Tdep_A	activation energy for processes caused by XA [J/mol]	75800
Tdep_KNHA	activation energy for factor KNHA for nitrification [J/mol]	-160000
Tdep_mueFB	activation energy for XFB growth [J/mol]	47800
Tdep_bFB	activation energy for XFB lysis [J/mol]	0
Tdep_AMB	activation energy for processes caused by XAMB [J/mol]	0
Tdep_ASRB	activation energy for processes caused by XASRB [J/mol]	0
Tdep_SOB	activation energy for processes caused by XSOB [J/mol]	0
Stoichiometric parameters		
$f_{Hyd,SI}$	production of S_I in hydrolysis	0.0
$f_{BM,SF}$	fraction of S_F generated in biomass lysis	0.05
$f_{BM,XI}$	fraction of X_I generated in biomass lysis	0.1
Y_H	yield coefficient for XH	0.63
Y_A	yield coefficient for XA	0.24
Y_{FB}	yield coefficient for XFB	0.053
Y_{AMB}	yield coefficient for XAMB	0.032
Y_{ASRB}	yield coefficient for XASRB	0.05
Y_{SOB}	yield coefficient for XSOB	0.12
Composition parameters		
$i_{N,SF}$	N content of S_F [g N/g COD_{SF}]	0.03
$i_{N,SI}$	N content of S_I [g N/g COD_{SI}]	0.01
$i_{N,XS}$	N content of X_S [g N/g COD_{XS}]	0.04
$i_{N,XI}$	N content of X_I [g N/g COD_{XI}]	0.03
$i_{N,BM}$	N content of biomass [g N/g COD_{BM}]	0.07
Oxygen		
cO2_sat_20	saturation concentration of oxygen [g/m³]	9.18
Tdep_cO2_sat	activation energy for saturation concentration of oxygen [J/mol]	-15000
rate_O2	re-aeration rate [1/d]	240

4. Geometry of the Transport Domain

The transport domain may be defined using relatively simple two-dimensional rectangular (Fig. 10) or three-dimensional hexahedral (Fig. 11) objects. In that case, the dimensions and other parameters of the transport domain are specified numerically using either the *Rectangular* (Fig. 10) or *Hexahedral Domain Definition* (Fig. 11) dialog windows. In both of these cases the transport domain is discretized into a structured finite element mesh. Alternatively, a more general two-dimensional geometry can be defined from basic boundary objects, such as points, lines, splines, polylines, arcs and/or circles. Boundary curves can consist of any combination of polylines, arcs, circles or cubical splines. The program permits one to specify internal boundaries (e.g., drains, wells, impermeable objects), as well as internal curves. A user can define from these boundary objects either a two-dimensional transport domain, the base plane (**base surface**) of the **three-dimensional layered domain**, or multiple surfaces that can then define the **three-dimensional general domain**. In the former two cases, the two-dimensional transport domain or the base plane of the three-dimensional domain is discretized into an unstructured finite element mesh.

4.1. *Boundary Objects*

The **computational domain** (the two-dimensional transport domain or the **base surface** of the three-dimensional domain) is formed by an arbitrary number of mutually nonintersecting **curves**. Each curve can be formed by connecting an arbitrary number of **objects**. Objects are defined by nodes, the positions of which can be specified either graphically with the mouse with possibilities to use **grid** alignment (Fig. 135) or by numerically defining their coordinates *X*, *Y*, and *Z*. It is also possible to read in the objects with a large number of nodes (**spline**, **polyline**) from a file containing the *x*-(, *y*-,) and *z*-coordinates for each node using the command *Insert->Domain Geometry->Points->Read from File* …. The order of inputting particular objects is arbitrary; the code automatically forms the desired curves. In order to have a physically realistic domain, only one closed outer curve can exists (for multicomponent domains such a curve must exist for each component of the domain). The domain can have an arbitrary number of **holes** or **internal curves**. The consistency of the geometry can be verified at any time using the command **Check Data Consistency** (**Tools Menu**). Any change in geometry can be undone using the **undo** command (up to ten levels backward in time) or redone using the **redo** command (again up to 10 levels).

An object type (e.g., polyline, spline, arc, or circle) must be selected first when designing a new object from the **Edit Bar** on the right side of the view window, or from menu (e.g., Insert->Domain Geometry->Nodes). Then points defining a particular object should be entered. The manner in which nodes are entered depends on the selected input style. When entering data graphically, an appropriate **Work Plane** (*x*-*y* *y*-*z*, *x*-*z*) and a grid with appropriately set parameters (Fig. 135 and Section 8.1.2) can be used to facilitate the input, while the coordinates *X*, *Y*, and *Z* of the cursor are continuously displayed in the bottom right corner of the window.

It is possible to edit existing objects by double-clicking on a particular object. The current selection, displayed in yellow, may be modified (edited) using the following operations: **delete**, **copy** (Fig. 52), **move** (Fig. 52), **rotate** (Fig. 53, left) and **mirror** (Fig. 53, right). Note that, in

addition to objects, particular nodes of an object can belong to a selected set as well, in which case the edit operations are carried out also for these points. Editing of selected objects (e.g., moving objects) also depends on the currently selected input style. The objects are moved with the cursor when the graphical mode is selected, while in numerical mode a vector of translation (*X*, *Y*, and *Z*) must be specified. It is possible to directly edit nodes of objects with the commands **insert point** (Fig. 44), **delete point**, and/or **move point**.

Before saving the data, an option is always displayed whether or not to verify the consistency of the geometry. We strongly recommend to regularly perform this test in order to prevent errors in subsequent calculations, e.g., during mesh generation.

Table 17. Definition of terms related to geometry design.

Objects

Objects are basic elements for building a geometric model of the computational domain and for defining other properties of the computational problem. Objects are divided into several categories (e.g., Geometry, FE-mesh, or Auxiliary), with each category containing several fields of objects of the same type. The shape (boundary) of the computational domain is defined using **Geometric objects**. Basic types of geometric objects are:

- points
- curves (polylines, arcs, circles, splines)
- surfaces
- openings
- thickness vectors
- solids

Points

A point is a basic geometric object which is used to define **Curves** and other objects. A point location is defined using two or three coordinates depending on dimensions of a particular problem.

Curves

A **curve** is a set consisting of a finite number of objects connected by boundary nodes. Except at point nodes, objects cannot intersect each other or themselves. A curve can be open or closed.

Outer Boundary Curves

An outer boundary curve is a boundary **curve** with the following properties: the curve is closed, positively oriented (i.e., in a counter-clockwise direction), does not intersect any other curve or itself, and has the computational domain (surface) located on its left side (in the sense of positive orientation), while the right side is not part of a computational domain.

Internal Curves

An internal curve must be located entirely within the computational domain. It can touch (but not intersect) the outside boundary of the computational domain at its definition points. An internal

curve can be open or closed, and can intersect itself, provided the intersect occurs at a definition point of the internal curve.

Openings

An opening is defined by one or more boundary **curves** that form a closed boundary.

Lines

Lines and polylines are the most commonly used objects for describing boundaries of a domain or internal curves. Lines are defined by two points specifying their beginning and end. Several lines can be connected to form "polylines" by connecting the beginning and end of two neighboring lines. Nodes can not coincide, while lines can not intersect each other.

Arcs

An arc can be defined either by a) **three points** on its circumference, b) a **center,** a **radius, two angles** (starting and final angle) and its orientation, and c) **two points**, a **center**, and a **radius**.

Circles

A circle can be defined either by **a center and a radius**, or by **three different points**.

Surface

A **surface** (the **computational domain** of two-dimensional applications) is defined by a finite number of continuous disjunctive bounded two-dimensional subdomains (Fig. 42). This means that the domain can be multicomponent, but that each of its components must have only one **outer boundary curve**. The domain can contain any finite number of **internal holes** or **internal curves**. **Surfaces** can be either **planar surfaces** (defined in a single plane) or **curved surfaces** (e.g., **Quadrangle**, **Rotary**, **Pipe**, or **B-Spline**). The **base surface** is a two-dimensional **planar surface** that can be extended into a three-dimensional **solid** (the **computational domain** of three-dimensional applications) using **thickness vectors**.

Thickness Vectors

The term **thickness vector** is used for a vector perpendicular to the **base surface** that extends the Base Surface to form a **solid** (three-dimensional **computational domain**).

Solids

The term **solid** represents a three dimensional **computational domain** that is formed either by the **base surface** and **thickness vectors** (**3D-Layered Solids**), or **boundary surfaces** (**3D-General Solids**), which can be either planar or curved (e.g., Quadrangle, Rotary, Pipe, or B-Spline).

Computational Domain

A Computational Domain is a continuous part of a two- or three-dimensional space for which water flow or solute transport is simulated. The **Domain Geometry** term relates to the shape of this space. The **Domain Geometry** can be defined for simple cases using parameters (using a Generalized Rectangle in 2D projects or a Generalized Hexahedral in 3D projects) and for general cases using boundaries (boundary curves for two-dimensional domains and boundary surfaces for three-dimensional domains).

In the **3D-Standard** version, the **Geometry** is defined using the **Base Surface**, which is a 2D domain of an arbitrary shape, and a set of **Thickness Vectors**, that define the variable thickness of the 3D domain or thicknesses of an arbitrary number of **Geo-Layers** (the term **Sublayers** was used in version 1, and is used alternatively in the text below). Such domain is then called the **3D-Layered** domain. Although such domains cannot be fully general, they allow definition of a majority of realistic 3D problems. In the **3D-Professional** version, the **Geometry** is defined using three-dimensional objects (Solids, bodies) of general shapes, which are formed by boundary surfaces, which can be either planar or curved.

A Computation domain can be formed using several surfaces that can touch each other, but can not overlap (Fig. 42). It is possible to create an opening in the base surface and then enter another surface into it. Division of the transport domain into individual surfaces enables easier work with it, since the program creates for each surface its own section and users can then specify different domain properties and initial and boundary conditions on these sections.

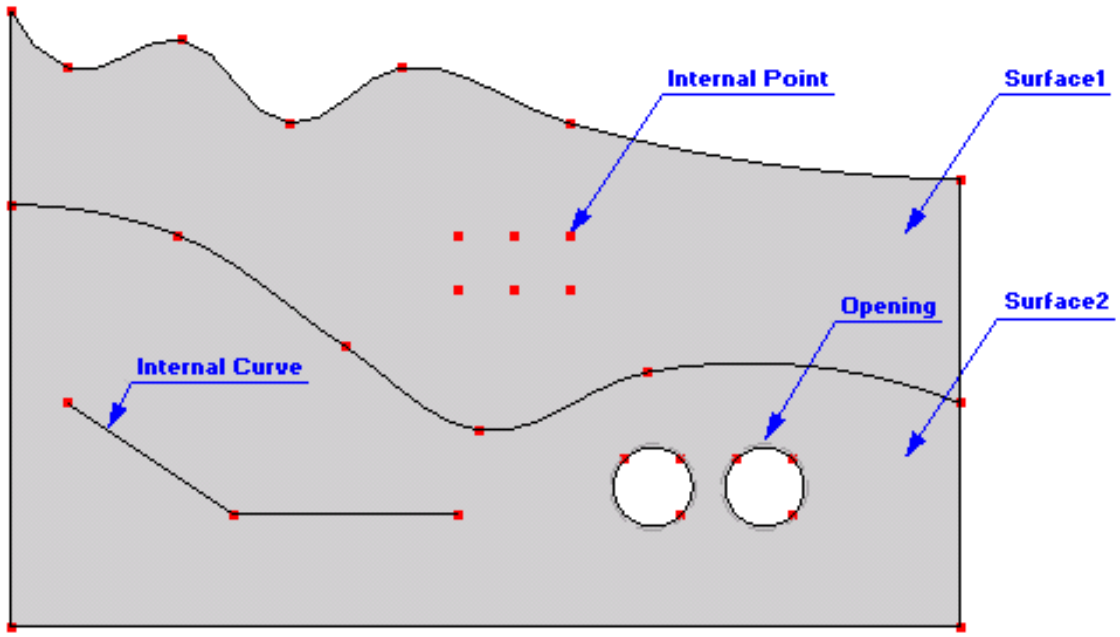


Figure 42. A base surface showing several basic geometric objects.

4.1.1. *Points*

Points can be either used to define **Boundary Objects** or can be located inside of the **Surface** (computational domain) and not be associated with any boundary object (**Single Points**). Points

can be entered either graphically using a cursor (most common) or using the **New Point** dialog window (identical to the **General Tab** of the **New Point** dialog, Fig. 44). To enter a new point graphically, select the command *Insert->Domain Geometry->Point->Graphically* from the menu, or **Points** from the **Insert Object** part of the **Domain Geometry** version of the **Tool Bar** at the right side of the **View Window**, and then enter the points using a cursor.

Once a command for defining a **new point** graphically is selected, a cursor in the **View window** will become a cross with a small empty circle in the middle. The coordinates of the location of the cursor will be displayed next to the cursor and on the **Edit Bar**, which will automatically change to the one displayed in Figure 43 (left). The **Edit Bar** will also show, which point (its number) is being defined and what reference coordinate system (the current coordinate system or the grid origin) is used. The process of defining new points is ended by pressing the Esc keyboard button, the right mouse button (see the **Help** part of the Edit Bar), or clicking the Stop button on the Edit Bar.

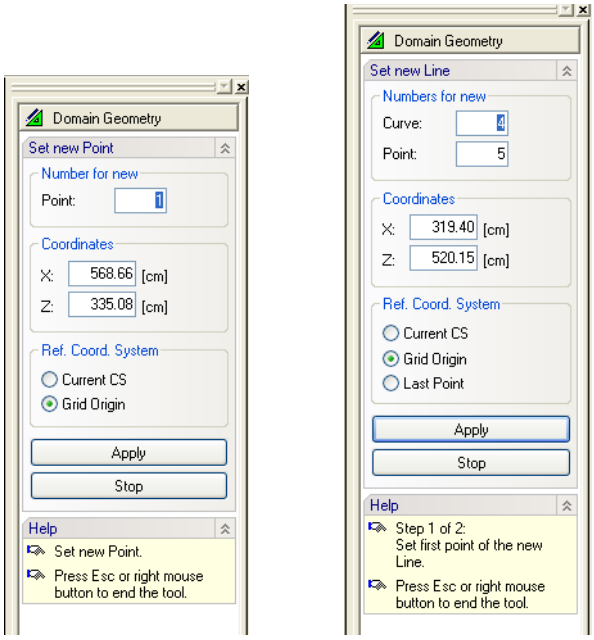


Figure 43. The Edit Bar during the process of defining graphically a new point (left) and a new line (right).

Double-clicking on an existing point will recall the **Edit Point** dialog window (Fig. 44). In addition to the **General Tab** (Fig. 44, left) in the **New Point** dialog window, the **Edit Point** dialog window has also the **FE-Mesh Tab** (Fig. 44, right). Coordinates of a point and its number are entered in the **General Tab**, while the **FE-Mesh Refinement** at a given point can be defined in the **FE-Mesh Tab**.

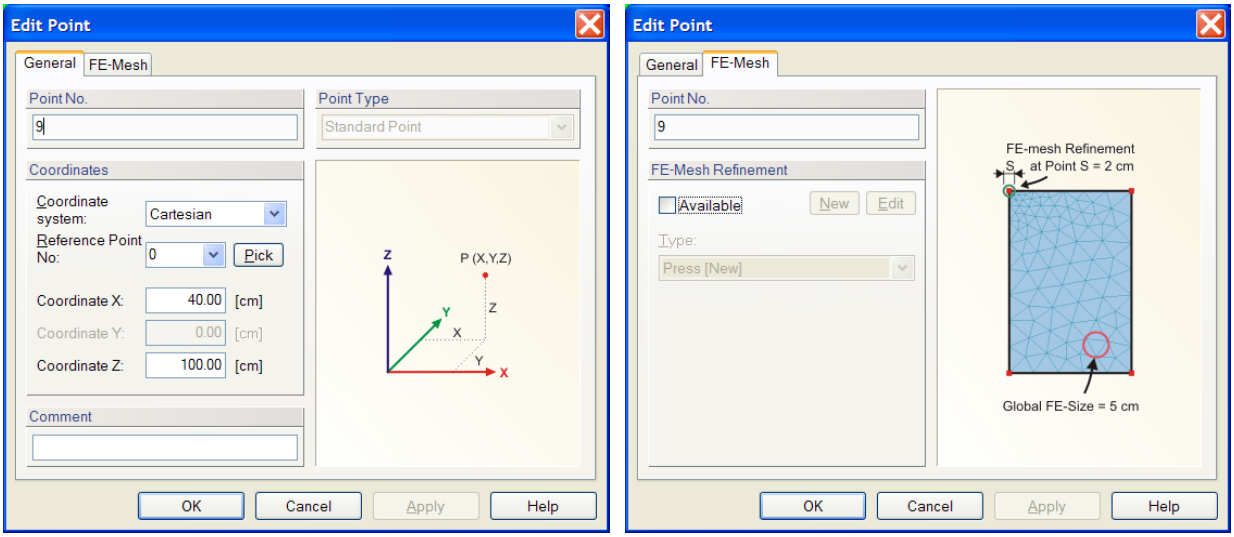


Figure 44. The Edit Point dialog window.

Although Cartesian Coordinates are usually used, it is possible to use also other coordinate systems:

Coordinate Systems in 3D Projects	Coordinate Systems in 2D Projects
• Cartesian • X-cylindrical • Y-cylindrical • Z-cylindrical • Spherical	• Cartesian • Polar

Reference Point: Point coordinates are usually related to the defined origin of the coordinate system. They can nevertheless be also related to another existing point, whose index is specified in the box **Reference Point No**. Locations of all related points are automatically adjusted when the location of the reference point is changed. The dependence of points on the Reference Point is, however, canceled during more complex operations, such as Copy, Rotate, or Drag and Drop. The coordinates of such points are then recalculated using absolute Cartesian coordinate system.

Point Type: Current version of HYDRUS recognizes two types of points:

- **Standard** – These are regular points defined using two or three coordinates.
- **Parametric** – These points are located on a curve and their location is calculated using a specified parameter from the interval (0.1), where 0 and 1 represent the beginning and end of the curve, respectively. For example, a point with a parametric coordinate t=0.5 is located exactly in the middle of the curve. A parametric point is not a defining point of a curve, i.e., it does not define its shape. On the contrary, a shape of a curve defines the location of a parametric point. A **Parametric Point** can be redefined as a **Standard Point** in the Edit Point dialog window (Fig. 44).

Parametric Points can be added on a curve using the command Insert Points on Line on the **Edit Bar**, using the menu command *Tools ->Insert Points On Line->Graphically*, or by clicking on a curve with the right mouse button and selecting the *Insert Points On Line->Graphically* from the popup menu (Fig. 45). Either the parametric coordinate of a point or its distance from boundary points (*L*) of a curve is displayed on the Edit Bar when specifying a **Parametric Point**.

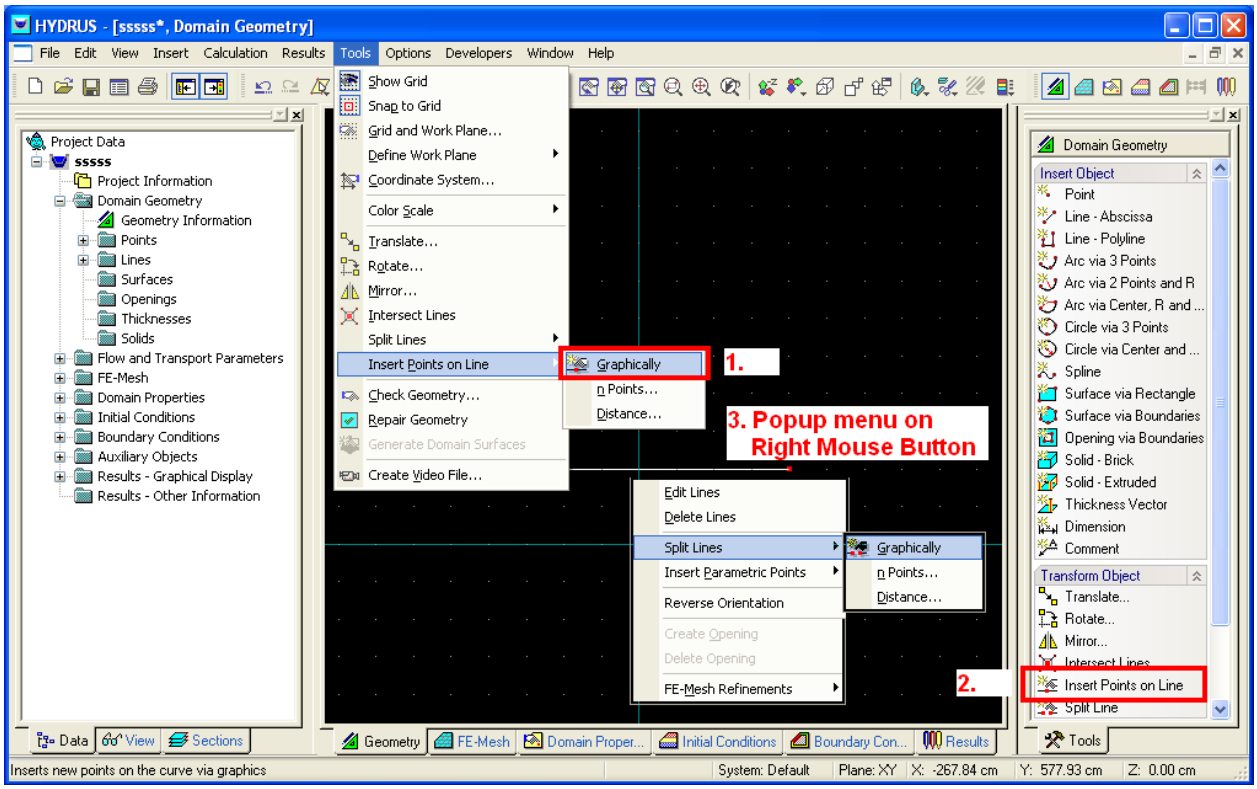


Figure 45. Different ways of adding Parametric Points on a curve.

4.1.2. *Lines and Polylines*

Lines and **Polylines** are the most commonly used objects for describing the boundaries of a two-dimensional domain and its internal curves. Similarly as above for **Points**, **Lines** and **Polylines** can be entered either graphically using a cursor (most common) or using the **New Line** dialog window (identical to the **General Tab** of the **Edit Line** dialog, Fig. 46). When entering a new line graphically, users can select the command *Insert->Domain Geometry->Line(Polyline)->Graphically* from the menu, or **Line - Abscissa** or **Line - Polyline** from the **Insert Object** part of the **Domain Geometry** version of the **Tool Bar** at the right side of the **View Window** and then enter the lines using a cursor.

Once a command for defining a **New Line** (a single abscissa) or a **New Polyline** is selected, a cursor in the **View window** will become a cross with a small empty circle in the middle. The

coordinates of the location of the cursor will be displayed next to the cursor and on the **Edit Bar**, which will automatically change to the one displayed in Figure 43 (right). The **Edit Bar** will also show, which point and curve (their numbers) are being defined and what reference coordinate system (the current coordinate system, the grid origin, or the last inserted point) is used. Once a single **Line** is specified (for a new line), one can immediately continue in specifying the second one, while the last point of the first line will be the beginning point of the second line. Each abscissa is considered to be a single curve. When a **New Polyline** is being created, the entire polyline is considered to be a single curve. The process of defining new lines is ended by pressing the Esc keyboard button, the right mouse button (see the **Help** part of the Edit Bar), or clicking the Stop button on the Edit Bar.

Double-clicking on an existing line will recall the **Edit Line** dialog window (Fig. 46). Before using the **New Line** dialog window, a user needs to first define points which are then used to define the line. In addition to the **General Tab** (Fig. 46, left) in the **New Line** dialog window, the **Edit Curve** dialog window has also the **FE-Mesh Tab** (Fig. 46, right). Points defining the line are entered in the **General Tab**, while the **FE-Mesh Refinement** along a given line can be defined in the **FE-Mesh Tab**.

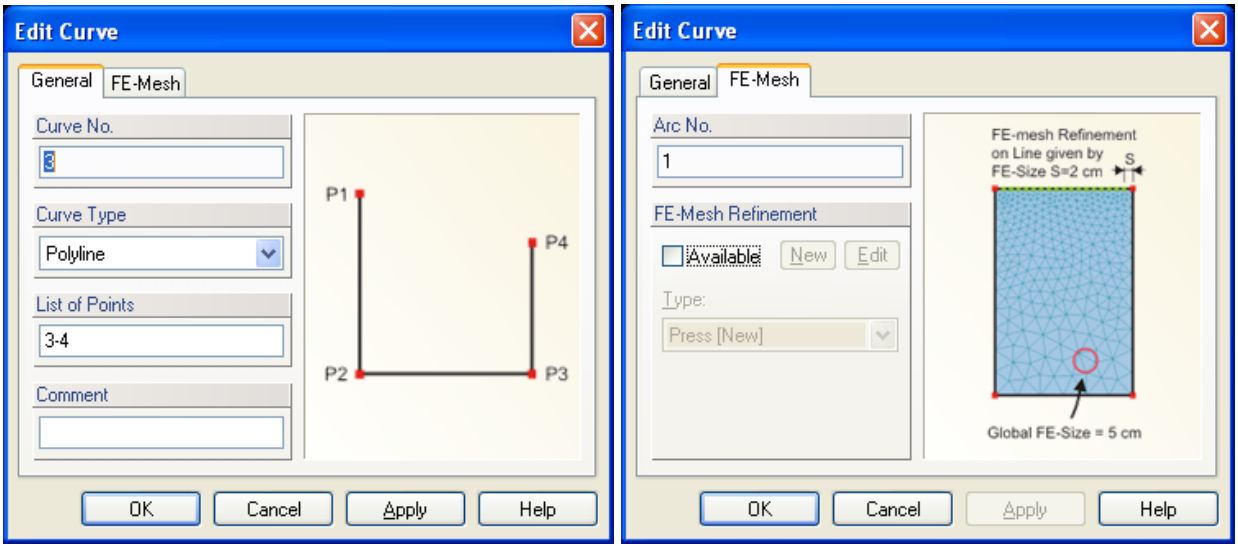


Figure 46. The Edit Curve dialog window.

4.1.3. *Arcs and Circles*

An **arc** is part of a **circle**. An object **arc** is always internally defined using three definition points. However, to simplify its specification, it is possible to define an **arc** graphically in multiple ways using: a) **three points** on its circumference, b) **a center, a radius, two angles** (starting and final angle) and its orientation, or c) by **two points**, a **center**, and a **radius**. Again, **arcs** can be entered either graphically using a cursor (most common) or using the **New Line** dialog window (Fig. 48). When entering a new **arc** or circle graphically, a user must select the command *Insert->Domain Geometry->Arc->Graphically* from the menu, or one of the following commands (a) **Arc by 3 Points**, b) **Arc by 2 Points and R**, or c) **Arc by Center, R and Angle**) from the **Insert Object**

part of the **Domain Geometry** version of the **Tool Bar** at the right side of the **View Window** and then enters **arc** using a cursor.

Graphical definition of **Arcs** and **Circles** is rather similar to the definition of **Points** and **Lines**. Differences occur when **Radii** or **Angles** are used to define these objects. For example, when user defines **Arc by 2 Points and Radius**, he/she first needs to define the two points, after which both the cursor and the **Edit Bar** change (Fig. 47, left) for the definition of the third type of information defining the arc. This can be a radius, an internal angle, or a height. The selection can be made on the **Edit Ba**r that also displays the magnitude of this variable (*R*, *A*) and a step (*dR*, *dA*) in which it can be increased.

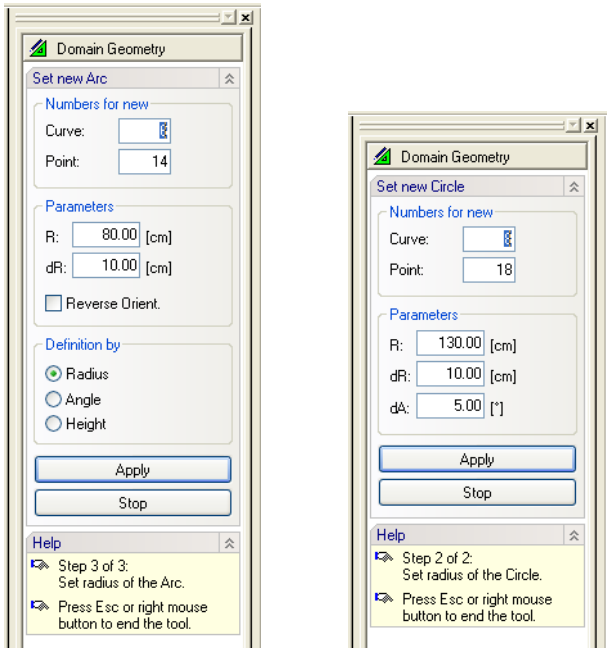


Figure 47. The Edit Bar during the process of defining graphically a radius for a new arc (left) or a new circle (right).

In addition to the **General Tab** (Fig. 48, left) in the **New Line** dialog window, the **Edit Line** dialog window has also the **Arc Tab** (Fig. 48, right). A list of points defining the arc are given in the **General Tab**, while coordinates of points defining the arc, its center and other parameters are entered in the **Arc Tab**. Double-clicking on an existing line will recall the **Edit Curve** dialog window (Fig. 48). The **Edit Curve** dialog window (Fig. 48) has an additional **FE-Mesh Tab** (similarly as for a line in Fig. 46; not shown here) where a user can refine the **FE-Mesh** along a given arc.

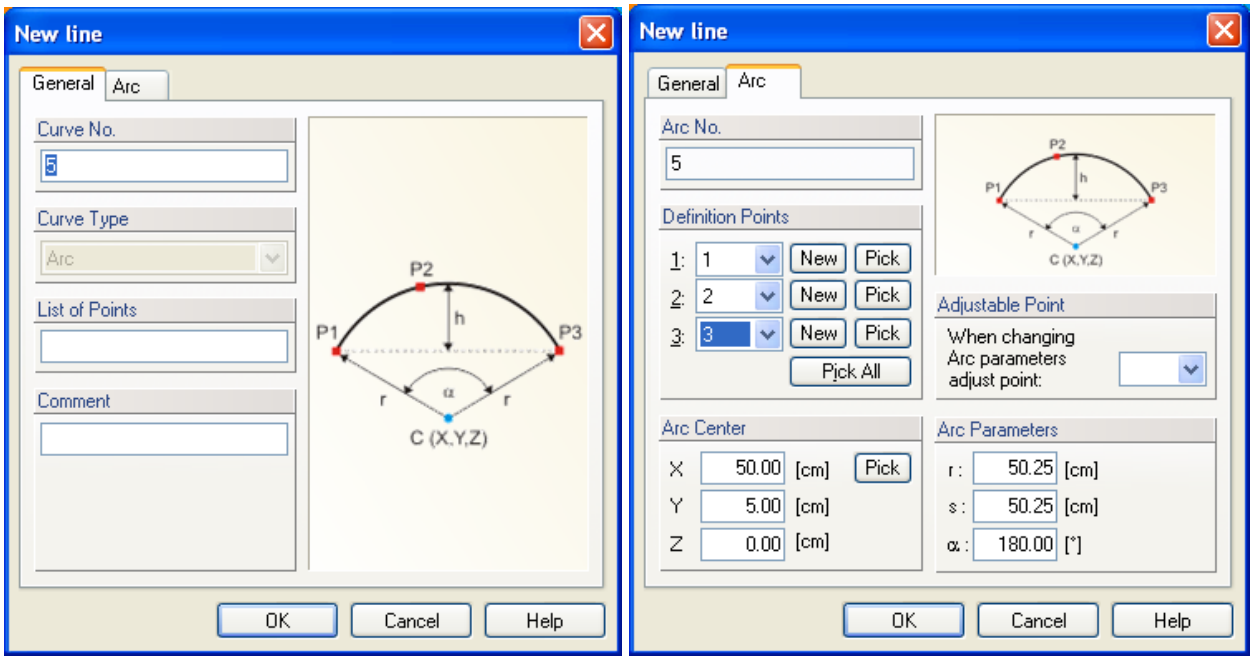


Figure 48. The New Line (Arc) dialog window.

An object **circle** is always defined internally using **three definition points**. However, to simplify its specification, it is possible to define a **circle** also using **a center and a radius**. Three definition points are then created automatically. Again, **circles** can be entered either graphically using the cursor (most common) or using the **New Line** dialog window (Fig. 48). A new **circle** can be entered graphically, by selecting the command *Insert->Domain Geometry->Arc(Circle)->Graphically* from the menu, or by using one of the following commands (a) **Circle by 3 Points**, or b) **Circle by Center and Radius**) from the **Insert Object** part of the **Domain Geometry** version of the **Tool Bar** at the right side of the **View Window**, and then entering lines using the cursor. The list of points defining the circle must be entered in the **General Tab** (Fig. 49, left), while coordinates of points defining the circle, its center and radius are entered in the **Circle Tab** (Fig. 49, right). When a **Circle** is defined **by Center and Radius** graphically, then the first definition point is created at the mouse click, while the other two are at the circle circumference at -90 and -180 degrees.

Adjustable Point: When a radius or the center of an arc is modified, it is usually also necessary to modify the location of one of the arc definition points. An adjustable point enables one to choose a point whose coordinates are to be changed.

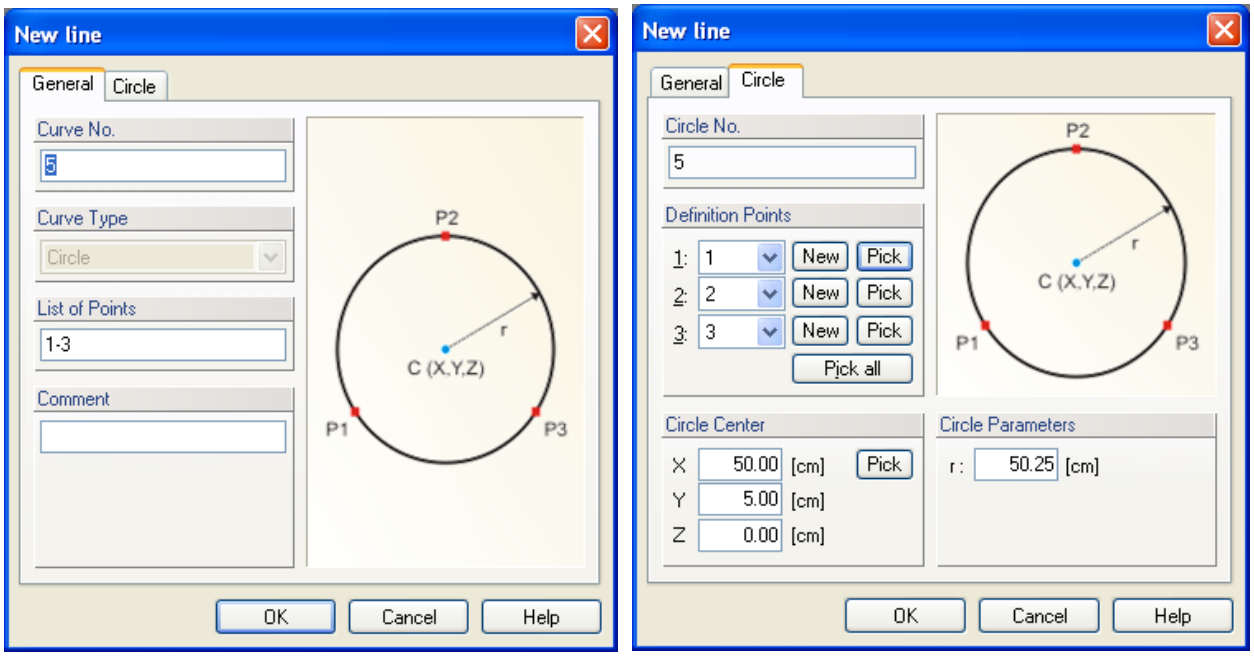


Figure 49. The New Line (Circle) dialog window.

4.1.4. *Curves and Splines*

The term "**Curve**" is used in the program and its documentation in two ways, while the meaning depends on where it is used.

1/ The term **Curve** is a general term for objects **Line**, **Polyline**, **Arc**, **Circle**, **Spline**.

2/ The term **Curve** can also refer to multiple objects (ad 1/) connected in their boundary points.

This meaning of the term **Curve** is mainly used in connection with "**Boundary Curve**", "**Internal Curve**", and so on.

There are several rules that need to be followed during the definition of a **Curve**.

- Curves cannot intersect each other or themselves except at their definition nodes.
- No point that is not either its definition or **Parametric Point** can lie on a **Curve**.

Curves are always defined using their definition points (their indexes). The list of indexes can be checked or changed using the **Edit Curve** dialog (the first Tab "General").

A **Spline** is a set of more than 2 points connected smoothly by cubic arcs. Splines are general smoothed curves defined using points in the 2D or 3D space. Three-dimensional splines do not generally have to lie in the same plane. However, if a spline is used to define a boundary of a surface, then all its definition points need to lie in this surface. A spline can be defined either

graphically using a command on the **Edit Bar** or in the dialog where we select a particular type of spline. HYDRUS allows three types of splines:

- cubic spline, i.e., a curve defined by multiple polynomials of the third order. It passes smoothly through all points.
- Bezier's curve – a smooth curve that passes through boundary points, but does not have to pass through internal points .
- B-spline – a general Bezier's curve.

More information can be found at
http://mathworld.wolfram.com/BezierCurve.html
http://mathworld.wolfram.com/B-Spline.html

Once a command for defining a **new spline** graphically is selected, a cursor in the **View window** will become a cross with a small empty circle in the middle. The coordinates of the location of the cursor will be displayed next to the cursor and on the **Edit Bar**, which will automatically change to the one displayed in Figure 50. The **Edit Bar** will also show, which point and curve (their numbers) are being defined and what reference coordinate system (the current coordinate system, the grid origin, or the last inserted point) is used. One node is specified after the other. A user can also select on the **Edit Bar** the type of the spline (standard spline, B-spline, or Bezier curve). The process of defining a new spline is ended by pressing the Esc keyboard button, the right mouse button (see the **Help** part of the **Edit Bar**), or clicking the Stop button on the **Edit Bar**.

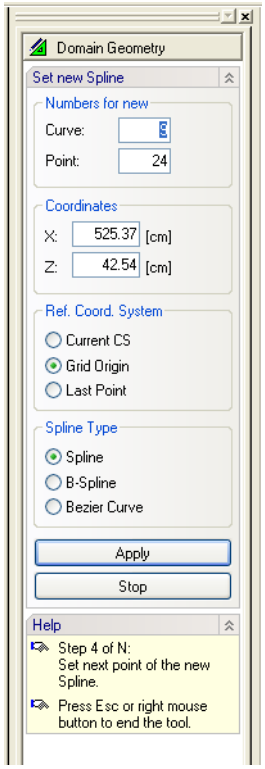


Figure 50. The Edit Bar during the process of defining graphically a spline.

4.1.5. *Common Information for a Graphical Input of Objects*

A/ A Numerical Input of Values. Edit controls displayed on the **Edit Bar** can be used to enter some values that are difficult to enter graphically as follows. Using a mouse one defines an approximate shape of an object. Then using a keyboard one enters selected values numerically. While entering values using a keyboard one can not move a mouse, or entered values will be lost. One needs to use the „Tab“ key or „Shift + Tab“ keys at the keyboard to move forward of backward from one edit controls to another one, respectively. A control of Combo Boxes and Radio buttons is done using a standard way as in dialog windows, i.e., using keys Arrow Up or Arrow Down, etc. After all values are entered one pushes the Enter key to finish the actual step of the running tool.

B/ Adjusting View. When graphically entering objects, one often needs to move or turn the scene, or to enlarge or reduce a selected detail. This can be done without interrupting the input of a particular object. The fastest way is to press the center mouse button (a wheel) and then a) dragging the scene with the mouse move, b) moving forward or backward an object by scrolling the wheel, or c) rotating the scene by simultaneously also pushing the right mouse button. After releasing the center mouse button, one can continue in the graphical input of an object. Similar operations can also be performed using button on the **View Toolbar**:

A majority of buttons on the View Toolbar do not interrupt the graphical input of an object, i.e., after the adjustment of the **View Window** on can continue in the graphical input of an object.

C/ Snapping. When entering Points graphically (points created when entering curves or surfaces), a process called **Snapping** is taking place. This means that a cursor snaps to points of a **Grid** (Fig. 51, left) or to existing points. **Snapping** can be disabled using a button **Snap to Grid** on the **Tools Toolbar**. **Snapping** on existing points or curves can not be disabled. **Snapping** occurs when a center of a cursor comes close to an existing point and when this point is redrawn with a yellow color (or any pre-select color assuming that redrawing of preselected points is not switched off). One can simultaneously observe on the **Edit Bar** that an index of a preselected point and its coordinates are displayed in edit controls. These controls are disabled since displayed values can not be changed. **Snapping** on curves (Fig. 51, right) occurs in addition to **Snapping** on existing points. An automatic calculation of coordinates of a point on a curve and snapping to this point occurs when a center of a cursor comes close to an existing curve. A location of this point is marked using a yellow cross which indicates that after this point is entered it becomes a definition point of a curve. This is important, since entering a point on a curve that is not its definition point leads to the wrongful definition of a domain. A **Check of a Geometry** discovers such errors and the **Repair Geometry** function will automatically correct it.

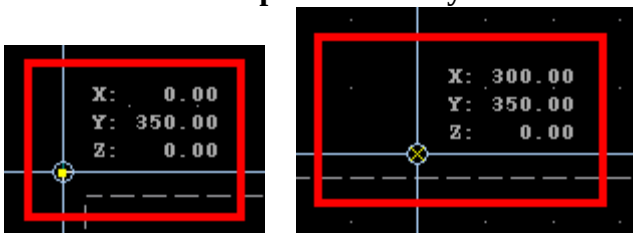


Figure 51. Snap to a point (left) and snap to a curve (right).

4.1.6. *Translate, Copy, Rotate, Mirror, Stretch, and Skew Operations*

All boundary objects can be manipulated using the **Translate**, **Copy**, **Rotate, Mirror**, **Stretch**, or **Skew** operations in the **Translate – Copy** (Fig. 52), **Rotate** (Fig. 53, left), **Mirror** (Fig. 53, right), **Stretch** (Fig. 54, left), and **Skew** (Fig. 54, right) dialog windows. These commands can be access either from the **Tools Menu** or from the **Transform Object** part of the **Domain Geometry** version of the **Tool Bar** at the right side of the **View Window**. Users first select an object to be manipulated, then click on the command, and specify the **Vector of Translation** for the **Translate** or **Copy** operations, or the **Angle of Rotation** for a **Rotation**, or define the **Mirroring Plane/Axis** for a **Mirroring** operation.

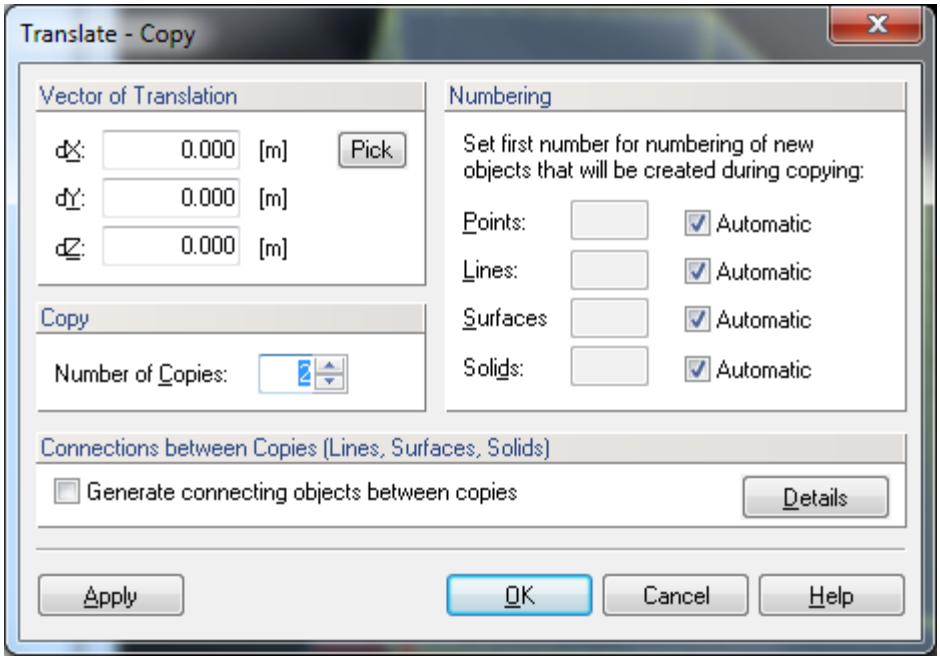


Figure 52. The Translate - Copy dialog window.

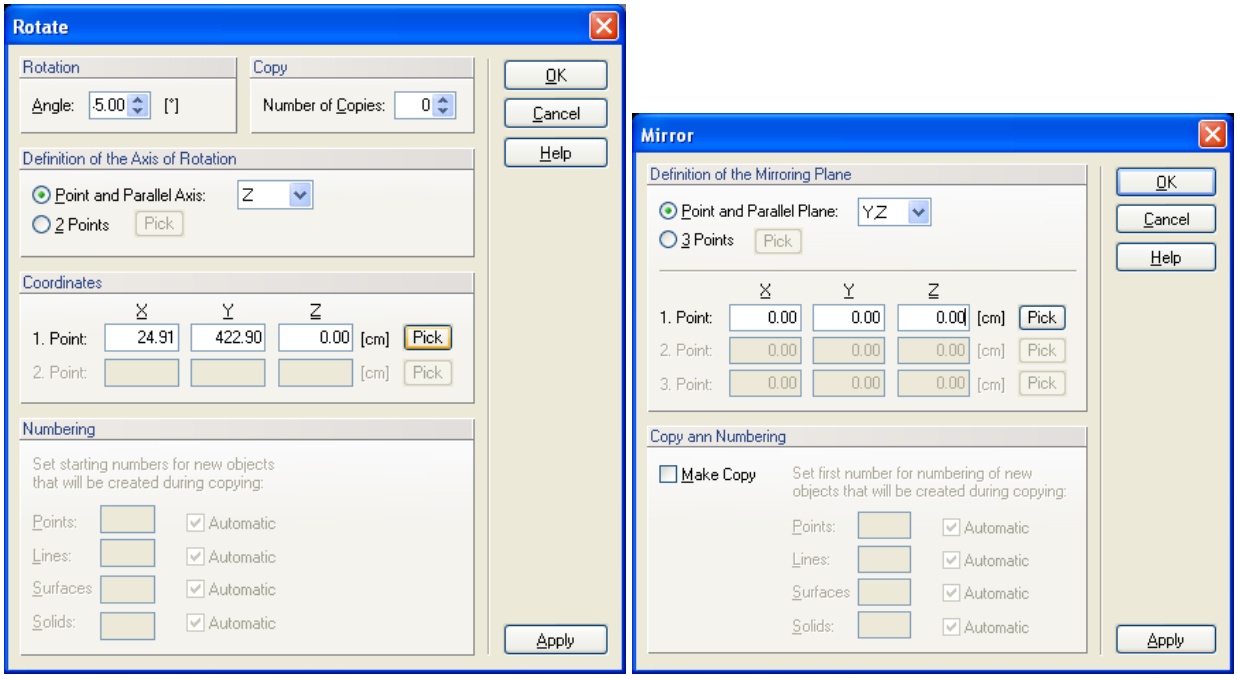


Figure 53. The Rotate (left) and Mirror (right) dialog windows.

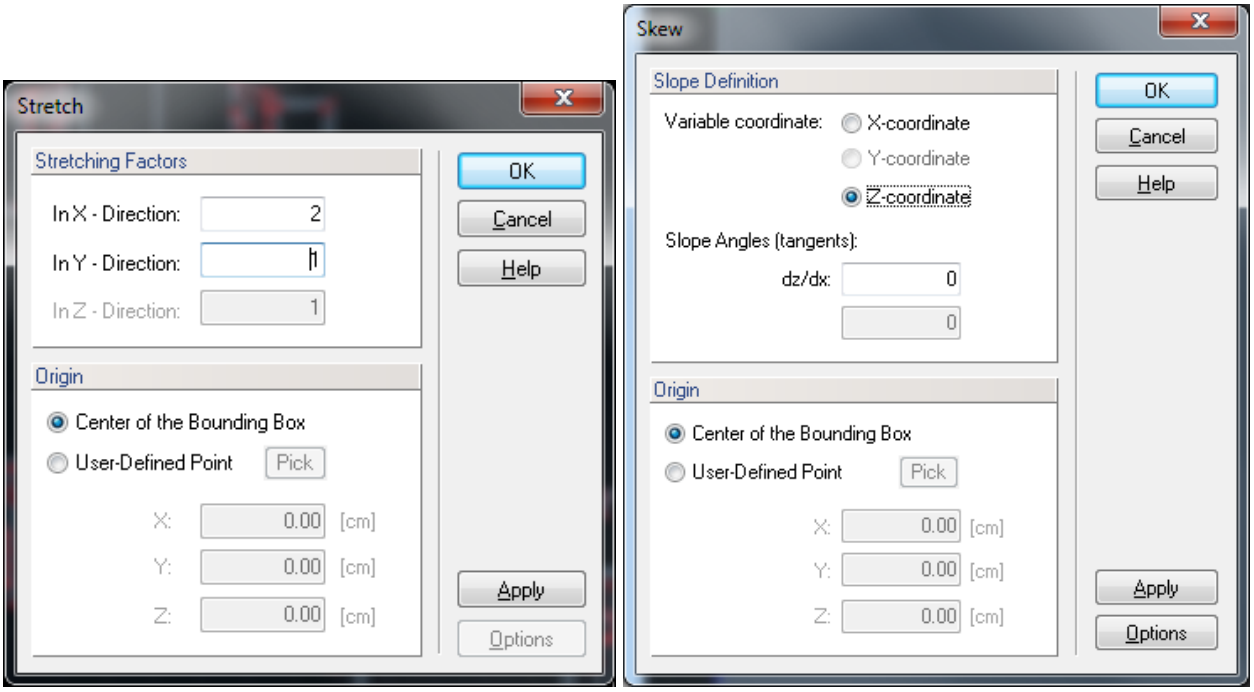


Figure 54. The Stretch (left) and Skew (right) dialog windows.

4.1.7. *Additional Operations*

Additional operations that can be used to manipulate boundary objects are **Intersect Lines**, **Insert Points on Line**, and **Split Line**. All three commands again can be accessed either from the **Tools** menu or from the **Transform Object** part of the **Domain Geometry** version of the **Tool Bar** on the right side of the **View Window**. The first command (**Intersect Lines**) finds the **Intersect** of two lines, whereas the second command **Insert**s **Points on** a **Line**. This can be done either graphically or numerically by specifying the number of nodes to be inserted on the line or distance of the point from the beginning of the line (Fig. 55). The third (**Split Line**) command can be used to split a line into two or more parts.

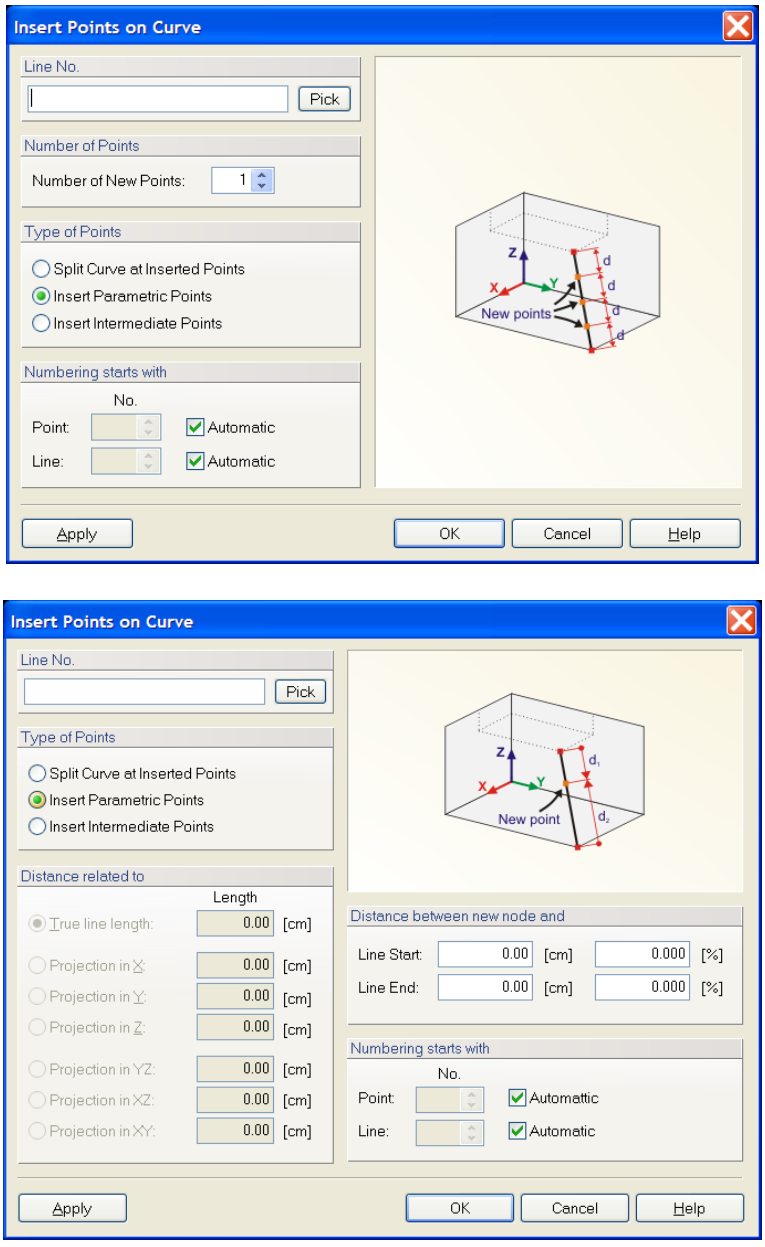


Figure 55. The Insert Point on Curve dialog window.

4.2. *Surfaces*

4.2.1. *General Definitions*

An object **Surface** refers to, depending on the problem type and the selection made in the **Domain Type and Units** dialog window:

- **2D-General:** For two-dimensional problems, a **Surface** serves to define the shape of the computational domain or its parts. See also **Geometry Information**.
- **3D-Layered:** In this case, the term **Surface** is used to define the **Base Surface** for **Solid - 3D-Layered** domains. This type of **Solids** is available in the **3D-Standard** version.
- **3D-General:** The term **Surface** serves to define boundary surfaces of a general 3D solid. This type of **Solids** is available only in the **3D-Professional** version. More detailed information can be found in the section about **Solid – General** (Section 4.4).

In the **3D-Standard** version, the only available type of a **Surface** is a **Planar Surface**. This type of the **Surface** is defined by its boundary curves that must all lie in the same plane and cannot cross each other. In the **3D-Professional** version, also the **Curved Surfaces** (**Quadrangle**, **Rotary**, **Pipe**, or **B-Spline**) are available.

A **surface** is a closed two-dimensional domain that is either the computational domain for two-dimensional applications or the **base surface** that can be extended into a **solid** for three-dimensional applications. A **surface** is defined by the **List of Boundary Curves**. It can be created using either the *Insert->Domain Geometry->Surfaces->Graphically* or *Insert->Domain Geometry->Surfaces->Graphically Rectangle* commands. Alternative commands on the **Insert Object** part of the **Domain Geometry** version of the **Tool Bar** are **Planar Surface via Rectangle** and **Planar Surface via Boundaries**. In the first case, a cursor appears and users can create a rectangular surface using the mouse. The **Edit Bar** displayed during this operation is similar to the one displayed in Figure 43 (right). The **Edit Bar** will also show, which point, curve, and surface (their number) are being defined. In the second case, users can create a surface by clicking on a closed curve (one or more boundary objects forming a close curve). The **Edit Bar** displayed during the operation will list **Boundary Curves** defining the **Surface** (Fig. 57, left). A **surface** can be edited using the **Edit Surface** dialog window (Fig. 57, right), which specifies surface type, the number of boundary curves defining the surface, its number, and had a box for possible comments or a description. A **surface** must be created before one can do finite element discretization.

A **Surface** can also be created automatically by using the menu command *Tools->Generate Domain Surfaces* or the **Edit Bar** command *Planar Surfaces - Generate*. After this command is clicked on, the program analyses existing boundary curves and attempts to generate planar surfaces automatically, i.e., without the user being required to define its boundaries. This operation is usually successful when there is a single uninterrupted boundary curve. The operation may fail when there are some ambiguities, such as when there are multiple curves or when boundary curves are not closed. If this operation fails, the following warning is displayed (Fig. 56) and the user needs to define Surfaces manually.

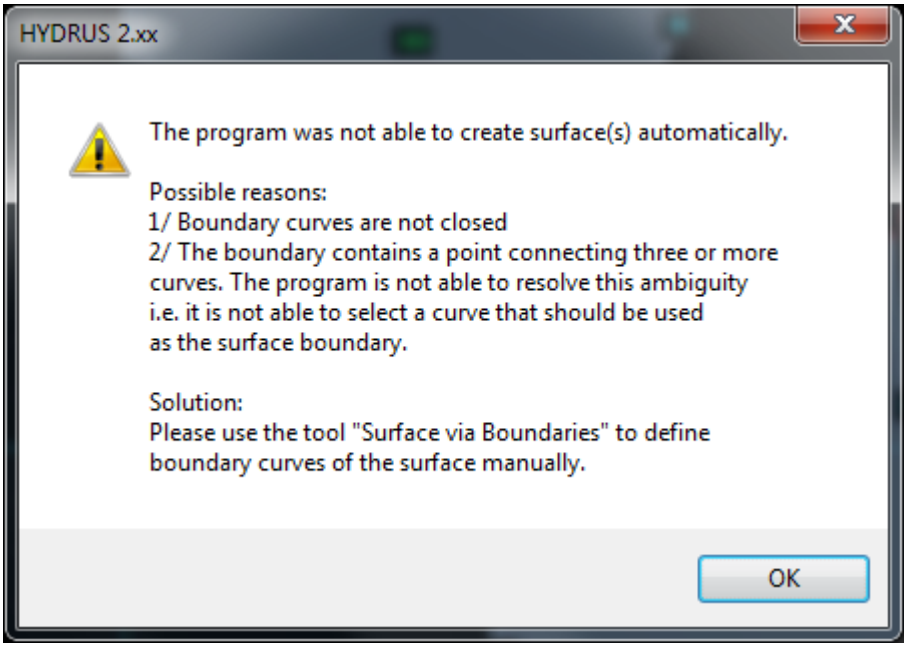

HYDRUS 2.xx
The program was not able to create surface(s) automatically.
Possible reasons:
1/ Boundary curves are not closed
2/ The boundary contains a point connecting three or more curves. The program is not able to resolve this ambiguity i.e. it is not able to select a curve that should be used as the surface boundary.
Solution:
Please use the tool "Surface via Boundaries" to define boundary curves of the surface manually.
OK

Figure 56. The warning issued when Surfaces cannot be created automatically and must be defined manually.

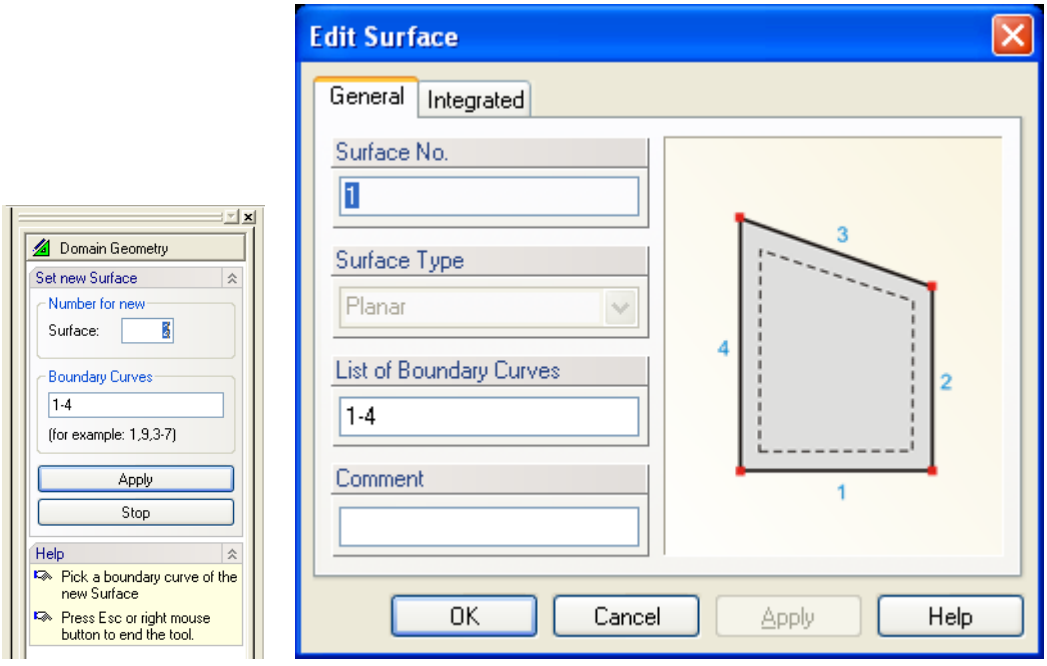


Figure 57. The Edit Bar during the process of defining graphically a surface (left) and the General tab of the Edit Surface dialog window (right).

4.2.1.1. *Planar Surfaces*

A **base surface** is formed by a **planar surface** of arbitrary shape. The base surface can contain **openings**, **internal curves**, and **internal points** (Fig. 58). In the current version of HYDRUS, a base surface can be formed by a single surface. Future versions will permit multiple surfaces to form one single base surface.

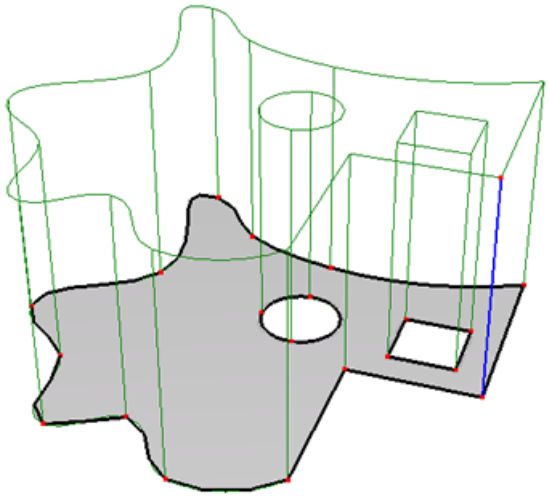


Figure 58. A solid showing the base surface.

If the solid needs to be divided into vertical columns, then these columns must be defined using internal curves in the base surface. The FE-mesh then follows exactly the specified shape of these internal curves (Fig. 59):

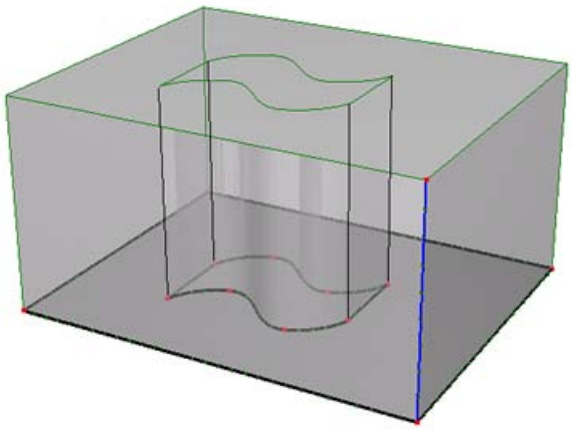


Figure 59. Solid showing separate vertical columns.

A **base surface** can be defined by a plane other than the horizontal plane, while thickness vectors can be defined in other than the vertical direction. Figures 60 and 61 show an example of a solid that has a base surface in the XZ plane and thickness vectors in the Y direction.

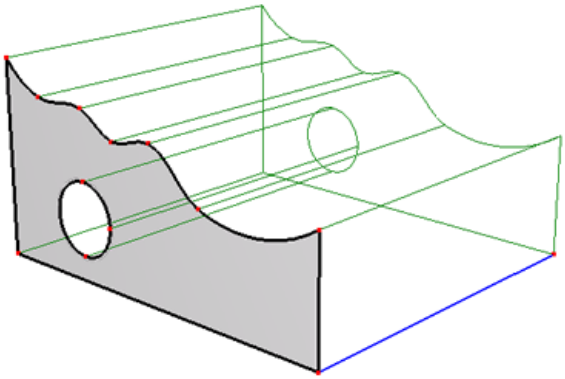


Figure 60. A solid with its base surface in the XZ plane and thickness vectors in the Y direction.

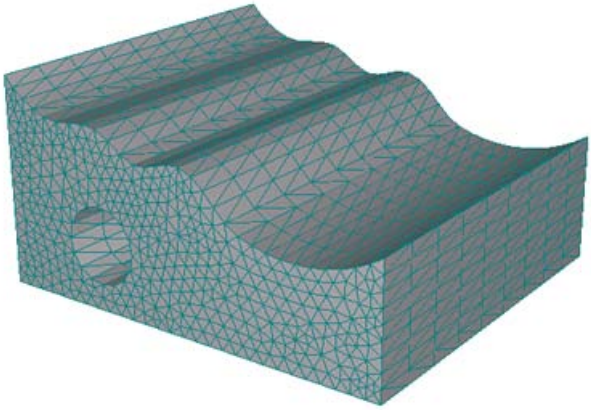


Figure 61. FE-Mesh for a solid with its base surface in the XZ plane and thickness vectors in the Y direction.

4.2.1.2. *Curved Surfaces*

There are currently four types of **Curved Surfaces** (Fig. 62) available in the **3D-Professional** version: **Quadrangle**, **Rotary**, **Pipe**, and **B-Spline**. While the boundary of a **Planar Surface** must be formed by multiple different **Curves**, the boundary of a **Curved Surface** can contain one curve two times. An example is a **Pipe Surface** (Fig. 62), in which the curve along a pipe occurs twice, each time with a different orientation. Note that the list of curves defining **Pipe** and **Rotary** Surfaces is generated automatically and cannot be edited, contrary to the list of curves defining **Quadrangle** or **B-Spline**, for which curves are selected by a user.

Quadrangle is a **Surface** defined by its boundary curves of an arbitrary type (except a circle). Curves do not have to be placed in a single plane, that is, in general, a **Quadrangle** can be a curved surface. This type of surface corresponds to a general surface with four corners, i.e., it is

typically defined by four boundary curves (although this is not a necessary condition). If there is another number of boundary curves than four, it is necessary to define corner nodes of a **Quadrangle**.

A **B-Spline Surface** is a **Surface** defined using **Boundary Curves** (similarly as a **Quadrangle**). However, for this type of **Surface**, one needs to also define additional matrix of *N***N* internal nodes, which allows one to curve the inside of a **Surface**. One needs to define a number of internal nodes *N* and an order of the **Surface Spline**. Internal nodes are created automatically when a **B-Spline Surface** is defined. Their coordinates can be subsequently edited. An order of the Surface Spline is an order of the polynomial, which is used for modeling the surface (either quadratic or cubic).

A **Rotary Surface** is defined by an **Axis of Rotation** (defined using two nodes), a **Rotated Curve** (of arbitrary type, as long as the created surface make sense), and an **Angle of Rotation** (from 0 to 360 degrees).

A **Pipe Surface** is defined by an **Axis Curve** (a smooth curve of an arbitrary type – only a polyline does not have to be smooth) and a radius.

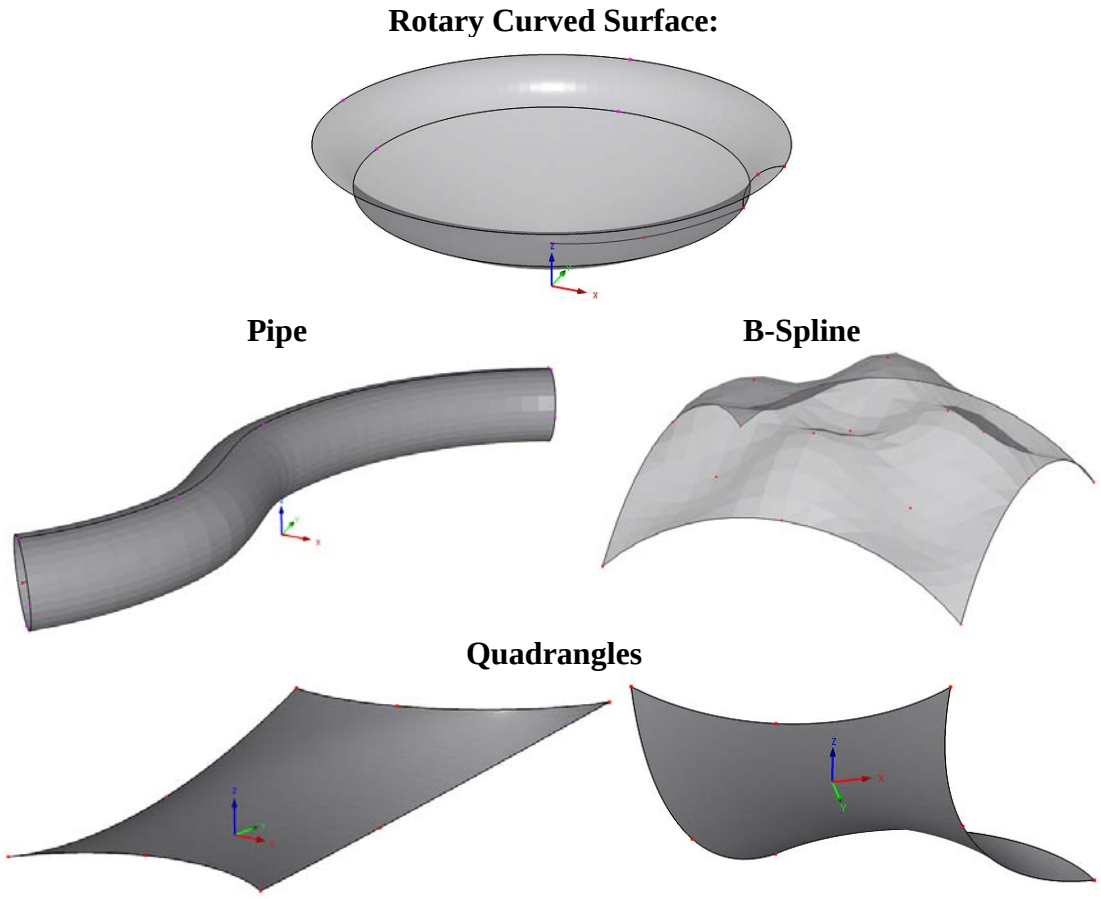


Figure 62. Examples of Curved Surfaces (Rotary, Pipe, B-Spline, and Quadrangle Surfaces).

4.2.1.3. *Partial Surfaces*

A **Partial** (or **Component**) **Surface** (Fig. 80) is created by an **Intersection of Surfaces** or **Solids** (see Section 4.6), which divides an original **Surface** into smaller **Sub-Surfaces**, or the so-called **Component Surfaces**. Although this **Surface** has its own number and can be used to define, for example, a **Solid**, its shape and boundaries are defined (generated) by the shape of its original **Surface** and a given **Intersection**. A list of **Components** resulting from division of the original **Surface** by an **Intersection** can be found on the **Tab Components** of the **Edit Surface** dialog window. Since **Partial Surfaces** are generated objects, they cannot be deleted or their shape cannot be edited (only the parental **Surfaces** can be edited). When a parental **Surface** is divided into **Components**, it still exists (is listed in the Navigator), but is not displayed in the **View** anymore; only its **Components** can be displayed.

One can define for each **Component** its activity (using commands **Activate Partial Surface** and **Deactivate Partial Surface**), i.e., whether it should be a part of the domain and whether a FE-Mesh should be generated on it or not. In this way one can cut from the original **Surface** unneeded parts. When an option „**Display components as independent surfaces**" is selected, **Components** are displayed in the **Navigator Data Tree** as independent **Surfaces** and it is possible to select them graphically and use them for a definition of **Solids**. A selected **Component** is displayed in a view, in order to facilitate visual identification of **Components**.

4.2.2. *Steps to Define a Two-Dimensional Domain*

1/ Definition of Boundary Curves of Particular Surfaces

Boundary Curves are formed using basic geometrical objects, such as **Points** and **Curves**. These objects can be specified in three different ways:

1. **Graphically.** One selects on the **Edit Bar** an appropriate tool and specifies new objects graphically in the **View Window**. This is usually done by specifying coordinates of points while using the **Grid Alignment** or snapping to already existing objects (points).
2. **Numerically.** Objects can be entered numerically by defining their *X*, *Y*, and *Z* coordinates and indexes in a dialog window. The dialog is obtained by using the **Menu** command *Insert –> Domain Geometry* or the **Navigator Bar** command *Data Tab –> Domain Geometry* and selecting the desired object type with a click of the right mouse button and the **New** command …
3. **Import from a File**. Particular objects (with a large number of nodes (**spline**, **polyline**) or the entire Geometry can be read from the text file using several formats. More detailed information is at **Read points from a text file** and **Import Geometry from a Text File**.

The order of inputting particular objects is arbitrary.

2/ Definition a Surfaces

Boundary Curves do not yet form the **Computational Domain**. The **Computational Domain** is formed using one or more **Surfaces** that need to be defined. A **Surface** is defined using a list of **Curves** that form a closed external boundary. A **Surface** can be defined **Graphically** by sequentially clicking on particular **Boundary Curves** or **Numerically** in a dialog where one can define a list of indexes of **Boundary Curves**.

3/ Internal Objects
Any surface can have an arbitrary number of **Openings** (**Holes)**, **Internal Curves** or **Internal Points**. Additional information can be found at **Internal Objects**.

4/ Openings
Each surface can have an arbitrary number of **Openings** (Holes). An **Opening** is defined by an closed internal boundary (one or more **Internal Curves**), which entirely lies inside of a **Surface**. An **Opening** can be formed by clicking with the right mouse button in the **View Window** on the closed internal boundary and selecting from the popup menu the "**Create Opening**" command. Additional information can be found at **Openings**.

5/ Geometry Check
The consistency of the geometry can be verified at any time using the command **Check Data Consistency** (**Tools Menu**).

6/ Remarks

- Any change in geometry can be undone using the **undo** command or redone using the **redo** command. A number of undo or redo step is limited by the buffer memory, which can be set in the **Program Options** dialog window (Tab **Options and Directories**).

- When the **Computation Domain** is formed by several subdomains with different properties (e.g., different materials and so on), one can form this domain from multiple **Surfaces** corresponding to these subdomain. An advantage is that after the **FE-Mesh** is generated, it is possible to automatically form **Mesh Sections** for particular **Surfaces** and use them to easily define materials and other properties or initial and boundary conditions. Additional information can be found at **FE-Mesh Sections** (Section 5.7).

4.2.3. *Several Notes on Rules for Correct Definition of Surfaces*

1. Contrary to the old HYDRUS-2D program, internal curves can touch or cross other internal curves and can touch boundary curves. A point where two curves intersect (or touch) must be a definition point of both curves (must be a part of the Geometry). This point can be found automatically using commands **Intersect Lines** (*Tools->Intersect Lines* or **Intersect Lines** from the Edit Bar) or **Repair Geometry** (*Tools->Repair Geometry*).
2. Curves cannot lie upon each other.
3. Multiple points can not be defined at the same location. A frequent error is when initial and final points of a curve are defined at the same location. The curve is then not closed and a surface can not be defined using this curve. Initial and final points of a closed curve must be

defined using the same point.

4. A point cannot lie on a curve without being its definition point.
5. All above mentioned errors in definition of the Geometry can be automatically solved using the command **Repair Geometry** (*Tools->Repair Geometry*).
6. Contrary to the old HYDRUS-2D program, the number of **Surfaces** is virtually unlimited (up to 30,000). **Surfaces** can touch each other (in a point or on a boundary line), or one Surface can lie inside of the other Surface. In this case one needs to first create an internal **Hole** in the first Surface and then insert the second Surface into this hole. This process can be recursive, i.e., it is possible to crease a Hole in the internal Surface and insert an additional Surface there). When defining a new Surface graphically (e.g., using a rectangle), HYDRUS recognizes when the new Surface is located inside of the existing Surface and automatically offers their integration.
7. Surfaces cannot partially cover each other (see also 6).
8. Points located outside of Surfaces are ignored when generating FE-Mesh.

4.2.4. *Internal Objects*

Internal Objects are objects of the type **Point**, **Curve**, or **Opening**, integrated in the **Surface** object. Objects are by default integrated into the Surface automatically (see Option "Autodetect" in Figure 1). It is possible to edit objects manually when the "**Autodetect**" option is turned off.
{bmct Internal_Object_Dlg.bmp}

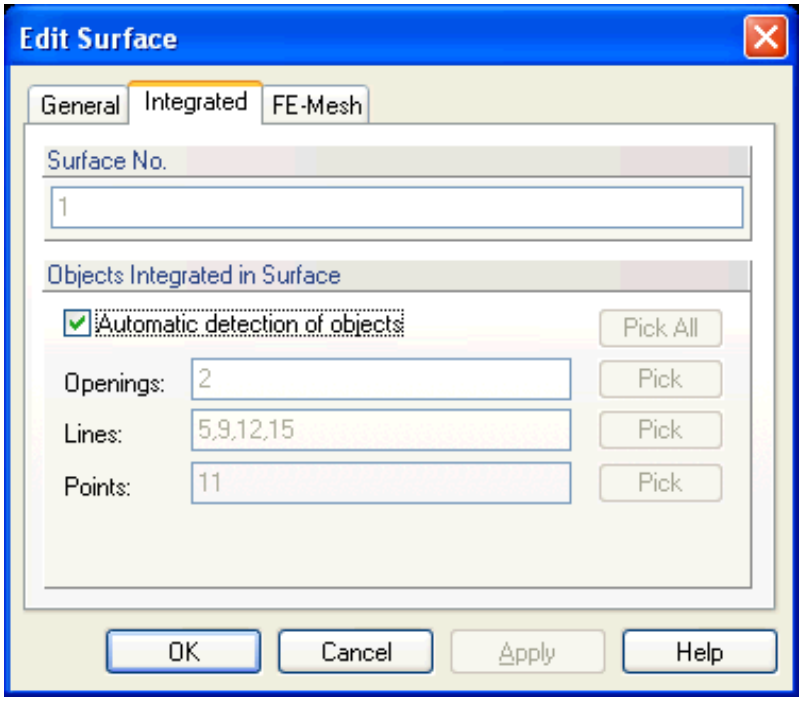


Figure 63. The Integrated Tab of the Edit Surface dialog window.

Main reasons for integrating objects into a **Surface**:

- Objects integrated in a **Surface** are respected when the FE Mesh is generated. On the other hand, objects that lie in a Surface but are not integrated in it are ignored during the FE Mesh generation.
- **Internal Points** allow users to precisely define location of **Observation Points** and other objects.
- **Internal Curves** allow users to precisely define geometrical boundaries inside of the transport domain. They can be used for many different purposes (e.g., **Mesh Lines**, Material Boundaries, etc).
- Curves integrated in a **Surface** that is used as a **Base Surface** for the **3D-Layered Solid** are projected also at the Upper Surface and enable thus more precise modeling of its shape (see Figs. 64 and 65).

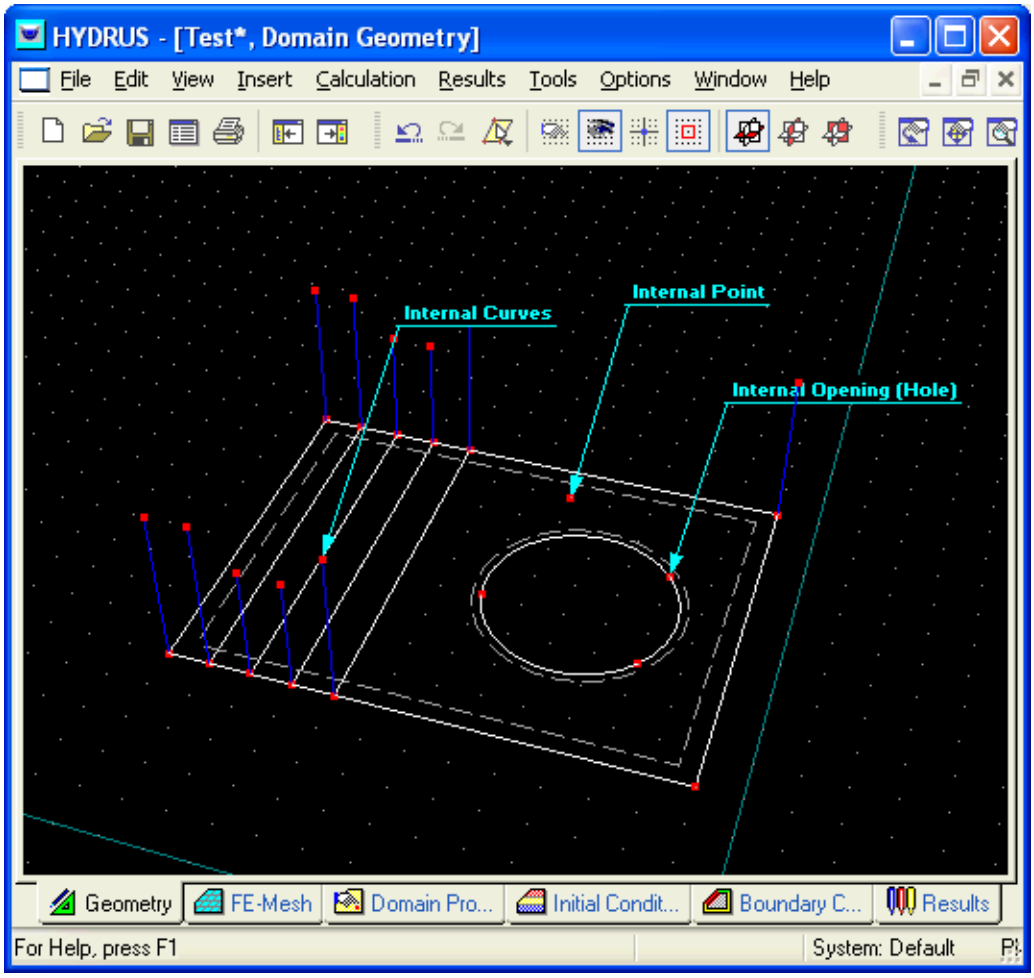


Figure 64. An example of internal objects.

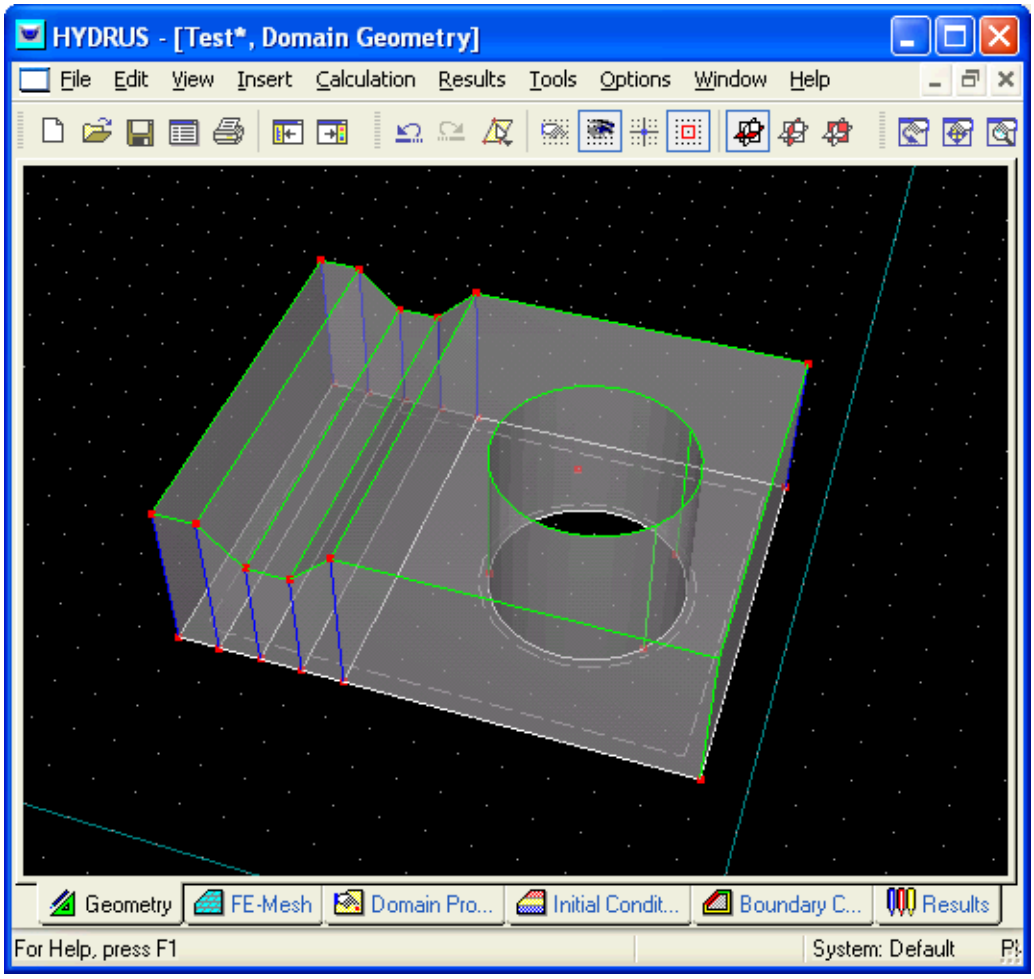


Figure 65. An example of an Upper Surface definition using Internal Curves and Thickness Vectors.

There are several rules that must be followed when defining **Internal Objects**:

- An **Internal Curve** must be entirely within a **Computational Domain**.
- An **Internal Curve** can touch (but can not intersect) the outside boundary of a parent **Surface** at its definition points (definition points of its boundary curves).
- An **Internal Curve** can be open or closed, and can intersect itself, provided that the intersect occurs at a definition point of an Internal Curve.

An **Internal Curve** or an **Opening** must lie entirely inside of the parent **Surface**. Common reasons why a **Curve** or an **Opening** are not automatically integrated into a **Surface** is that there exist small deviations between them and a **Surface** that are not visible, but are larger than allowed tolerance (usually 0.1 mm).

4.2.5. *Check and Repair Geometry*

The **Check Data Consistency** command performs a consistency test of the domain boundaries. It checks especially whether each domain component is bounded by an outer boundary curve and whether or not the curves are intersecting each other. When the geometry is not correct, the code sends a warning and select those curves which do not fulfill he rules for a correct definition of boundaries. The command **Repair Geometry** may then be used to fix existing problems.

The **Repair Geometry** command attempts to fix errors in the ill-defined **Geometry** that were found using the command **Check Data Consistency**. This command calls the **Repair Domain Definition** dialog window (Fig. 66). The **List of Corrections** section of this dialog lists various operations that can be used automatically by the program when attempting to correct the ill-defined **Geometry**. Some of these corrections depend on the model precisions, which are defined in the **Model Precision and Precision of Corrections** section. Users can define these precision criteria or use those suggested by HYDRUS.

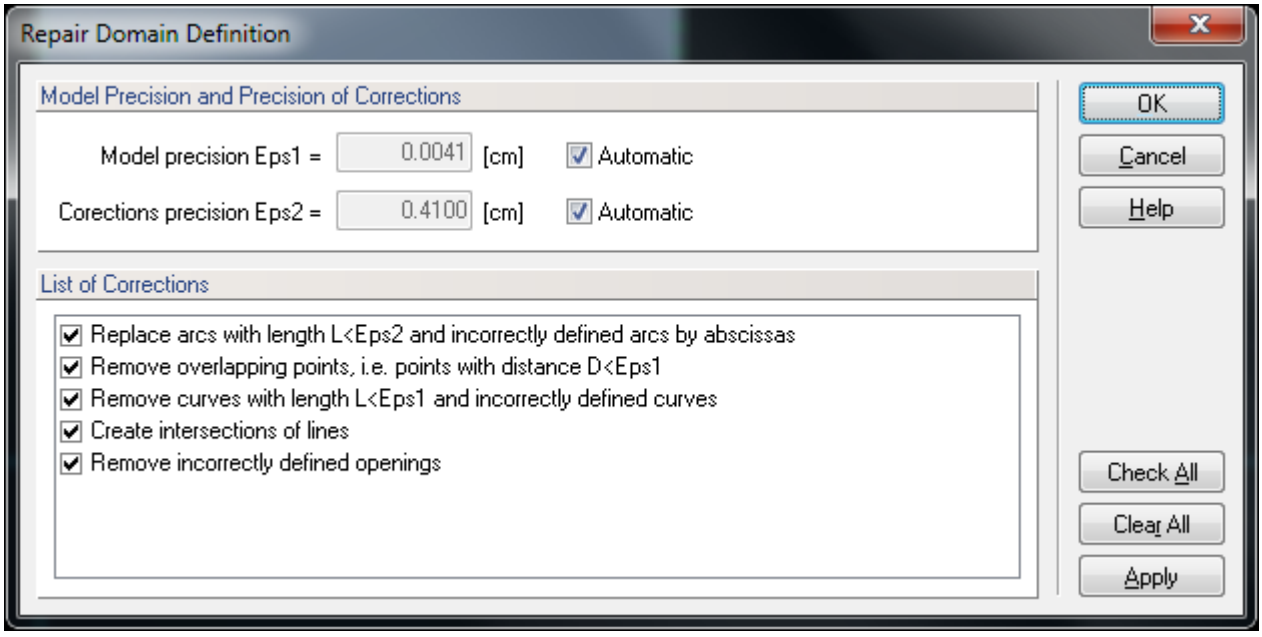


Figure 66. The Repair Domain Definition dialog window.

4.3. *Opening*

An **opening** is an internal hole defined by a **boundary curve** having the following properties: the curve is closed, positively oriented (in a counter-clockwise direction), does not intersect any other curve or itself, and has the computational domain located on its right-hand side (in the sense of positive orientation), while the left side is not part of a computational domain. An **opening** is not part of the computational domain or surface. An **opening** is created graphically as follows: One first defines boundary objects that create a closed boundary curve. One then uses the command *Insert->Domain Geometry->Opening->Graphically* from the menu, or alternatively the command **Opening via Boundaries** on the **Insert Object** part of the **Domain Geometry** version of the **Tool Bar**. A user creates an **opening** by clicking on the closed curve (one or more boundary objects forming a closed curve). The **Edit Bar** displayed during the operation will list **Boundary Curves** defining the **Opening** (similar to Fig. 57, left). Alternatively, an **opening** can be created using the **New Opening** dialog window (Fig. 67) by clicking on the command *Insert->Domain Geometry->Opening->Dialog* from the menu. An **opening** can be edited using the **Edit Curve** dialog window (Fig. 46), which specifies the number boundary curves defining the opening, its number, and has a box for possible comments or a description.

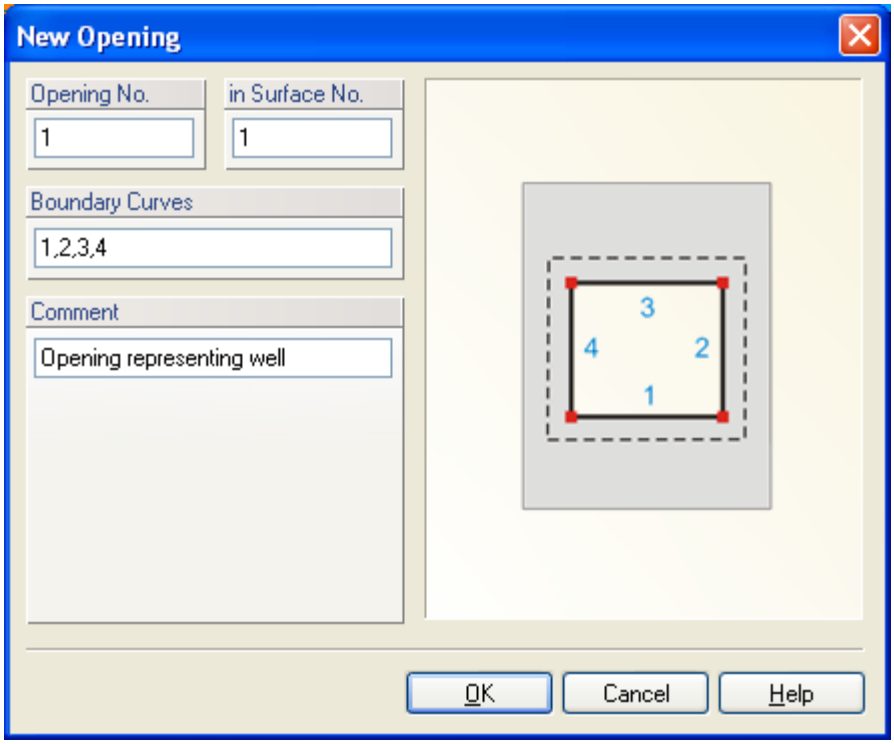


Figure 67. The New Opening dialog window.

4.4. *Solids*

Solids are three-dimensional objects defined by the **base surface** and one or more **thickness vectors** (See also Section 2 - **Projects** Geometry Information). There are three types of Solids depending upon the selection made in the **Domain Type and Units** dialog window (Figs. 6 and 7):

- **3D-Layered – Hexahedral:** This type of solid has a **Hexahedral Shape** and is defined by its basic dimensions (Figs. 6 and 9). The base can have a certain slope in the X and Y dimensions.
- **3D-Layered – General:** This type of solid is defined by the Base Surface and one or more **Thickness Vectors**.
- **3D-General:** This type of solid is defined using a set of surfaces (either **Planar** or **Curved Surfaces**) that form its boundaries. This selection is available only in the **3D-Professional** version of HYDRUS.

4.4.1. *3D-Layered – Hexahedral Solids*

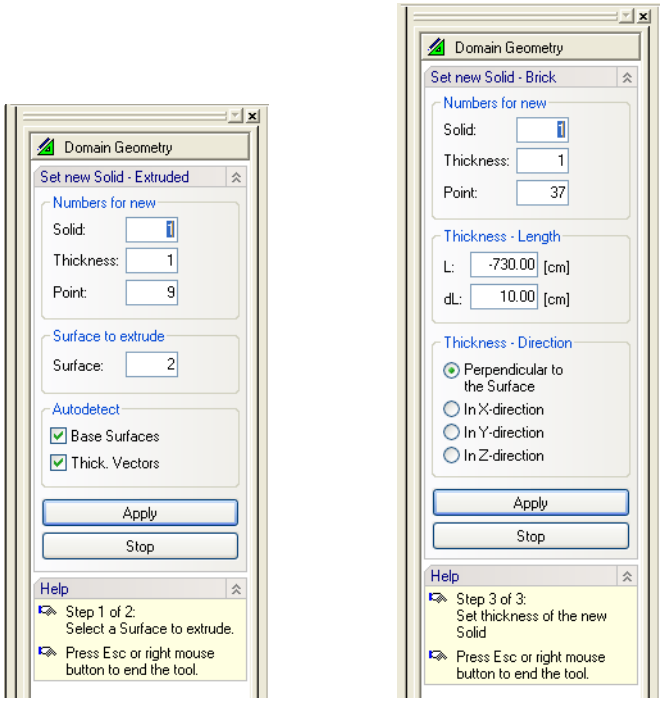


Figure 68. The Edit Bar during the process of graphically defining a Hexahedral Solid. Definition of a Base Surface on the left and a Thickness on the right.

A simple **Hexahedral Solid** can be created graphically using the menu command *Insert->Domain Geometry->Solid->Graphically* or alternatively the command **Solid - Extruded** on the **Insert Object** part of the **Domain Geometry** version of the **Tool Bar**. Once a command for

defining a **new Hexahedral Solid** is selected, a cursor in the **View window** will become a cross with a small empty circle in the middle. The coordinates of the location of the cursor will be displayed next to the cursor and on the **Edit Bar**, which will automatically change to the one displayed in Figure 68 left. The **Edit Bar** will also show, which point, curve, and surface (their numbers) are being defined and what reference coordinate system (the current coordinate system, the grid origin, or the last inserted point) is used. After two points defining a surface are specified, both the cursor and the **Edit Bar** change (Fig. 68 right) for the definition of the Thickness Vector. The selection can be made on the **Edit Ba**r that also displays the height of the Thickness Vector (*L*) and a step (*dL*) in which it can be increased. The Thickness Vector can be created (a) Perpendicular to the Base Surface, b) in X-direction, c) in Y-direction, or d) in Z-direction). The process of defining a new Hexahedral solid is ended after the Thickness Vector is defined.

4.4.2. *3D-Layered – General Solids*

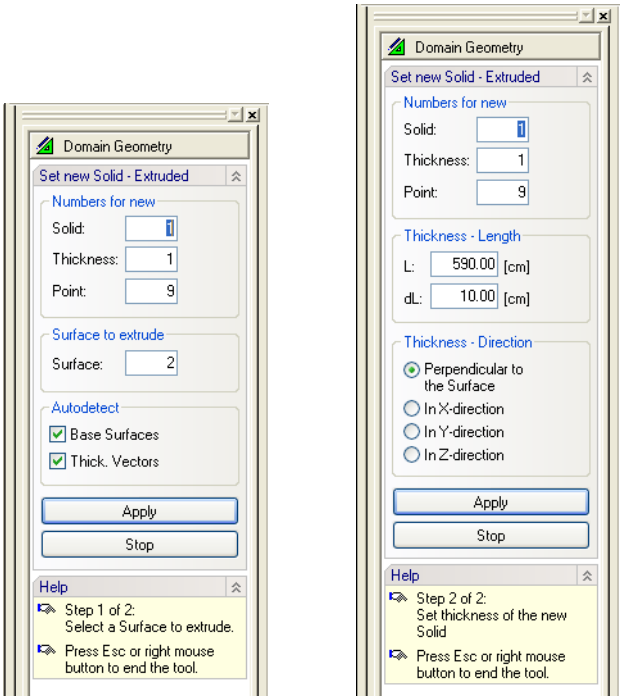


Figure 69. The Edit Bar during the process of graphically defining a Solid by extruding a Base Surface. Selection of a Surface (left) and definition of a Thickness Vector (right).

A **Solid** can be created graphically (*Insert->Domain Geometry->Solid->Graphically* from the menu or alternatively the command **Solid - Extruded** on the **Insert Object** part of the **Domain Geometry** version of the **Tool Bar**) by clicking on one point defining the **Base Surface** and extruding the base to form a three-dimensional solid. During the first part of the operation the **Edit bar** (Fig. 69 left) displays numbers for a Solid, a Thickness Vector, a Point, and a Surface, while during the second part it (Fig. 69, right) displays the Thickness Vector length (and increment) and in which direction it is created (a) Perpendicular to the Base Surface, b) in X-direction, c) in Y-direction, or d) in Z-direction). A user should during the first step select (click

on) the **Base Surface** that is to be used to define the **Solid**. It is also possible to click on any **Point** that defines the **Base Surface**. The second step depends on whether **Thickness Vectors** are already defined in **Points** of the **Base Surface**. If they are, they are used to define the **Solid** and the second step is not done. If they are not, the thickness of the solid needs to be defined during the second step. The length and direction of the **Thickness Vector** is defined using a mouse in the Point on the **Base Surface** closest to the mouse click which selected it.

How to create a **Solid** once the **Base Surface** and multiple **Thickness Vectors** are defined?

1. Graphically: Use the "**Solid Extruded**" tool and click on the **Base Surface**. A **Solid** is created using existing **Thickness Vectors**.
2. Numerically: By using a command from the **Insert** menu or by clicking with the right mouse button on **Solids** in the **Data** tree of the **Navigator Bar**. From the popup menu select the **New Solid** command. In the **New 3D-Layered Solid** dialog select the **Base Surface** and **Thickness Vectors**. Since the **Autodetect** function is automatically on, the **Base Surface** and **Thickness Vectors** will likely be detected automatically.

Thickness vectors do not have to be perpendicular to the **base surface**. A **Solid**, i.e., its **base surface** and **thickness vectors**, is defined and can be edited in the **Edit Solid** dialog window (Fig. 70) that has four tabs: **General**, **Sub-Layers**, **Thickness Profiles**, and **FE-Mesh**. The **General Tab** provides information on which **base surface** and which **thickness vectors** define the solid. The **Sub-Layers Tab** informs whether the solid is divided into one or more **Layers**. **Layers** are other objects that can be used to subdivide a single solid. These layers can be used, for example, to keep constant thicknesses of selected horizons or constant discretization close to the soil surface (to get good estimates of evaporation) across the entire transport domain (solid). Layers can have different **Thickness Profiles** (**the Thickness Profiles Tab**). One profile is created by the code automatically. Users can then define one or more **Thickness Profiles** that are associated with different **Thickness Vectors**. These profiles can then be subdivided into multiple layers that can have either constant or variable thickness (**T**) across the transport domain. Thicknesses and the mode (constant or variable) of particular layers are specified in a table. Thickness Sum (**TS**) is then calculated by adding thicknesses of particular layers. At least one layer thickness must be variable. The finite element discretization then follows these layers. Finally, the **FE-Mesh Tab** (Fig. 71) specifies how many horizontal FE-Layers are used to discretize the solid. When only one layer exists then users can specify relative finite element spacing (spacing of vertical discretization layers) on the vertical side (*FE-Mesh Layer Spacing*) using the RS1 (relative size at the top) and RS2 (relative size at the bottom) factors below *Generate Mesh Layer Spacing*. The element sizes are then proportionally distributed. The preview part of the dialog window shows the main terms used on each Tab. When multiple layers exist then users can specify relative sizes of elements for each layer (*FE-Mesh Density in Layers*).

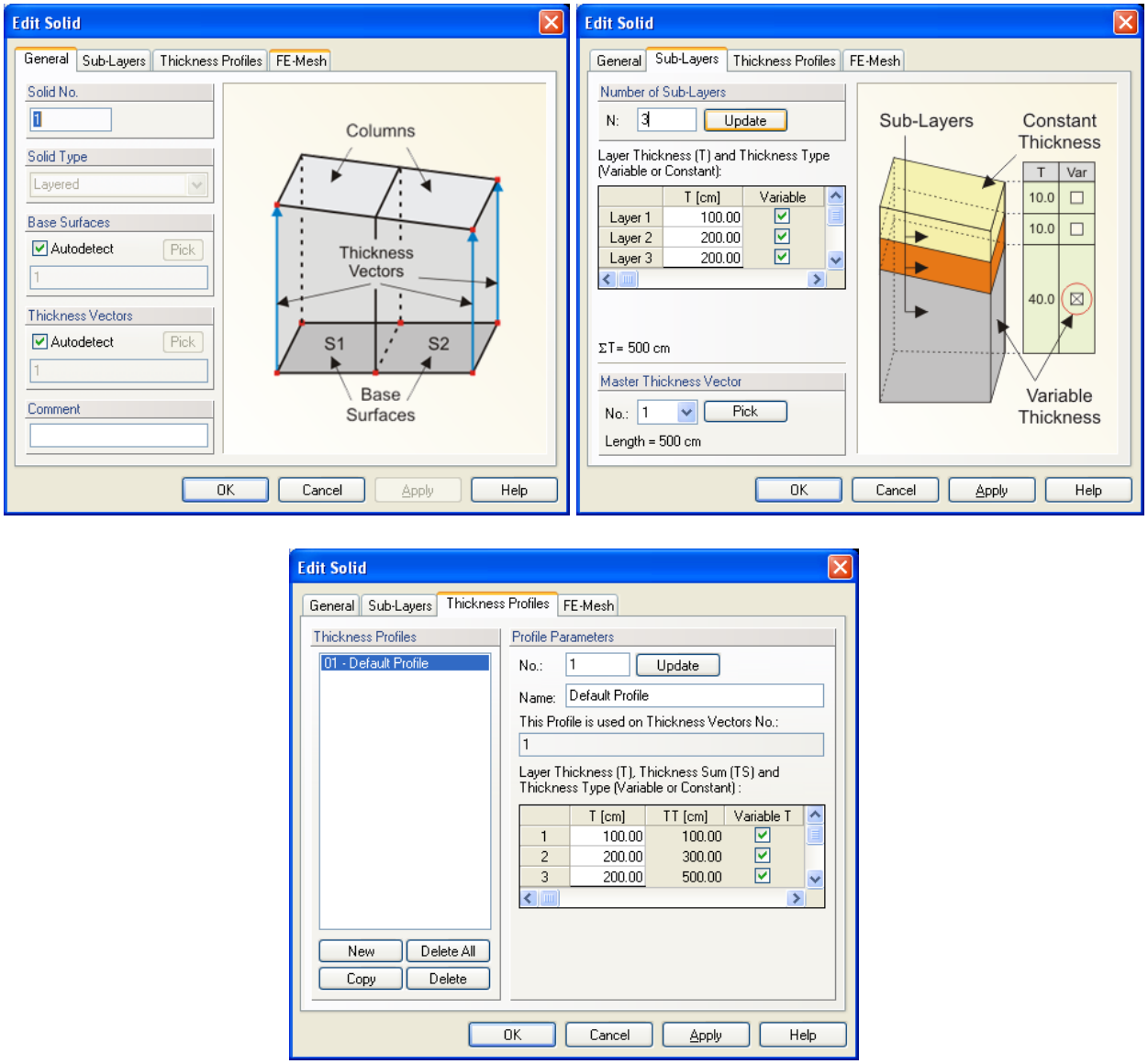


Figure 70. The Edit Solid dialog window; the General, Geo-Layers, and Thickness Profiles Tabs.

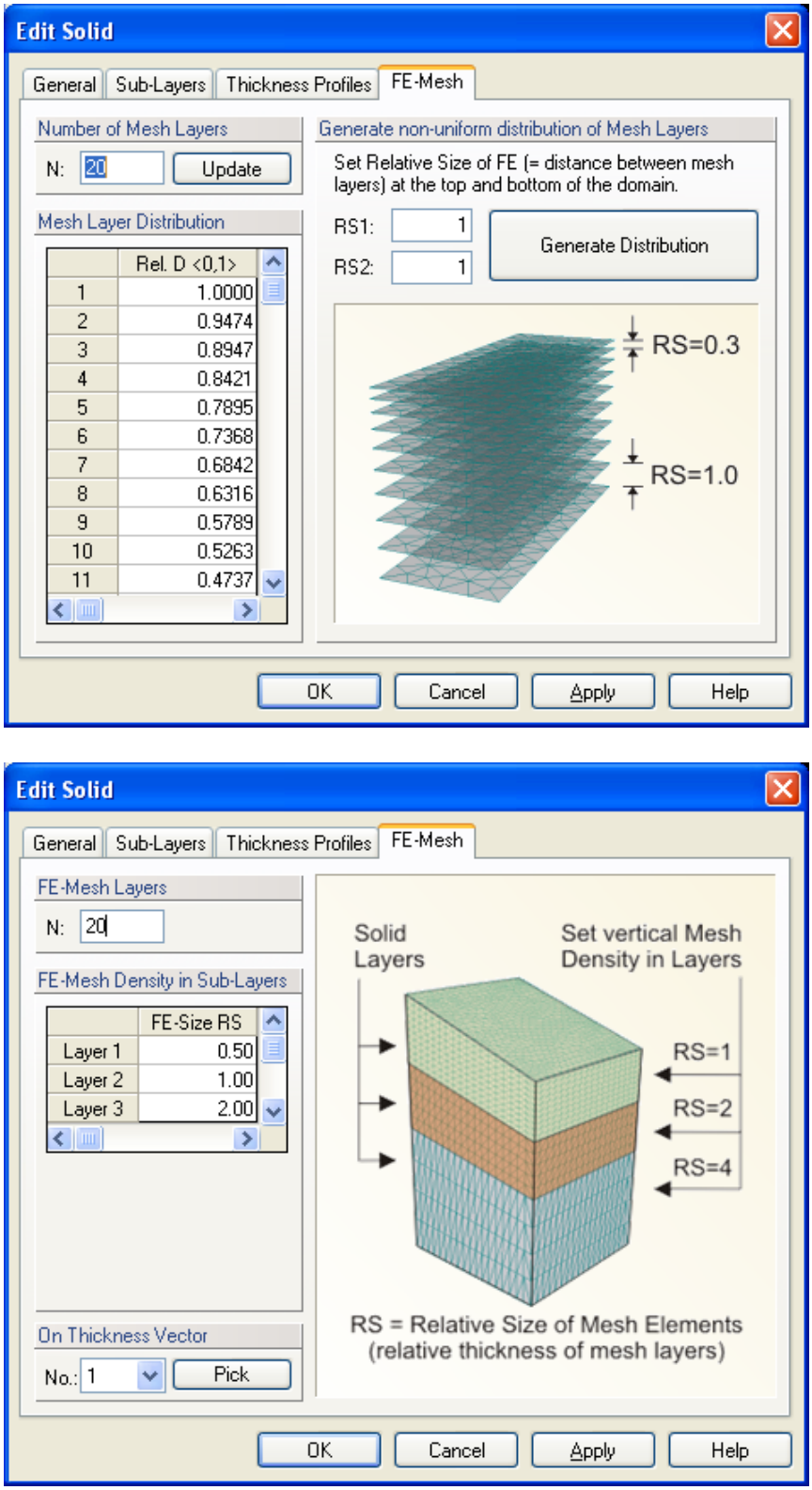


Figure 71. The Edit Solid dialog window; the FE-Mesh Tab for a single and multiple layers.

4.4.2.1. *Division of a Solid into Columns*

Notice that the **Base Surface** must be defined using several **Surfaces** (see Fig. 58). Parts of the **Solid** above each **Surface** are called **Columns** and serve to geometrically divide the **Solid** in the vertical direction. All **Surfaces** defining the **Base Surface** must lie in a single plane. A list of these **Surfaces** can be defined manually using indexes or can be **Autodetected** by the program (the "**Autodetect**" option). A division of a **Solid** into **Columns** leads to an automatic creation of **Mesh Sections** that correspond with **Columns** after the generation of the **FE-Mesh**. These **Mesh Sections** can be used to define various properties (e.g., materials distribution) or initial and boundary conditions.

4.4.2.2. *Division of a Solid into Geo-Layers*

Geo-Layers (alternative term **Sublayers**, which was used in Version 1 is used alternatively below) are used to divide a **Solid** in the horizontal direction (Fig. 70).

It is possible in the **Edit Solid** dialog to define number of **Layers** and their **Thicknesses**. A **Solid** has always one **Master Thickness Vector**, which is one of **Thickness Vectors** of a **Solid**, that has a special meaning as described below.
A thickness of a **Layer** is calculated as follows:

- **Thicknesses of Layers** given in the Table are calculated on the **Master Thickness Vector**
- The sum of **Thicknesses of all Layers** should be equal to the length of the **Master Thickness Vector**. If it is not so, a program will issue a warning and recalculate **Thicknesses of Layers** automatically.

A **Solid** can have more **Thickness Vectors** of different lengths so that specified **Thicknesses of Layers** cannot be maintained. The program then does the following: For **Geo-Layers** with the **Constant Thickness Type**, the specified thickness is maintained at all **Thickness Vectors**, i.e., over the entire computational domain. For **Geo-Layers** with the **Variable Thickness Type**, their thicknesses are linearly increased or decreased so that the sum of **Thicknesses of all Layers** corresponds with the length of a particular **Thickness Vector**.

4.4.2.3. *Individual specification of different Thicknesses of Geo-Layers at different Thickness Vectors.*

In the preceding paragraph we have described how to define **Thicknesses of Layers** on the **Master Thickness Vector** using a table (Fig. 70). This table represents the so called **Profile**, i.e., a particular distribution of thicknesses. If one wants to define precisely the division of thicknesses also on other vectors than the **Master Thickness Vector**, then it is necessary to create additional **Special Profiles** and use then on corresponding **Thickness Vectors**. There is always a **Default Profile**, which corresponds to the table described in 4.4.2 above. One can create new profiles, change their thicknesses or delete them. One can simultaneously also see a list of **Thickness Vectors** where the selected **Profile** is used.

A desired **Profile** can be associated with a particular **Thickness Vector** after opening a dialog with its properties (e.g., by double clicking on a vector) and selecting a **Profile** from a Combo Box "**Thickness Profile No.**" (see Fig. 74). This operation can even be carried out globally by first selecting desired **Thickness Vectors**, then opening a dialog with their properties (Alt + Enter), and finally repeating the above described process. Note that one **Profile** can be associated with many **Thickness Vectors**, which enables one to change easily **Thicknesses of Layers** on all **Thickness Vectors** by changing a single **Profile**.

4.4.2.4. *Steps to Define a 3D-Layered Domain*

1/ Definition of the Base Surface

The **Base Surface** is a **2D domain of an arbitrary shape**. How to specify the **Base Surface** is described in **Building a Two-Dimensional Domain.**

2/ Definition of Thickness Vectors

One inserts one or more **Thickness Vectors** in points that lie in the **Base Surface**, so that the shape of a **Solid** is defined as needed.

3/ Definition of a Solid

On the **Edit Bar** (or the Menu command *Insert –> Domain Geometry*) one clicks on the ***Solid –> Extruded*** command and selects (clicks on) one of the **Surfaces** defining the **Base Surface**. This operation creates the **3D-Layered Solid**. One can do this even when no **Thickness Vectors** are defined. In such case after clicking on the **Base Surface** a graphical tool is started, using which one can extrude the **Solid** into the space. A **Thickness Vector** is simultaneously created in the **Point** on the **Base Surface** that is closest to the location of the click.

4/ Formation of a Solid

A **Solid** can be further formed using additional **Thickness Vectors** and **Internal Lines**.

5/ Definition of Geo-Layers

A **Solid** can be vertically divided into **Layers.**

4.4.3. *3D-General Solids*

Solids in the 3D-Professional version are defined using boundary **Surfaces** (either **Planar** (see Section 4.2.1.1) or **Curved** (see Section 4.2.1.2)) and identified as **3D-General Solids**. In one project, one cannot use at the same time **3D-General Solids** and **3D-Layered Solids** (created in the 3D-Standard Version) or the parametric blocks (created in the **3D-Lite Version**). It is,

however, possible to convert **3D-Layered Solids** into **3D-General Solids** by changing the project type from **3D-Layered** to **3D-General**.

Boundary Surfaces of a **Solid** must enclose a closed space and cannot intersect each other. Interior of a **Solid** must form a three-dimensional "simply continuous space", i.e., it must be possible to connect any two internal points using a polyline that is entirely located inside of a **Solid**. Boundaries of a **Solid** thus can be formed by any number of either **Planar** or **Curved Surfaces**. Figure 72 shows two examples of 3D-General solids. While the **Solid** at the top is formed using 8 **Planar Surfaces** and 4 **Quadrangles**, the **Solid** at the bottom is formed by multiple **Curved Surfaces**.

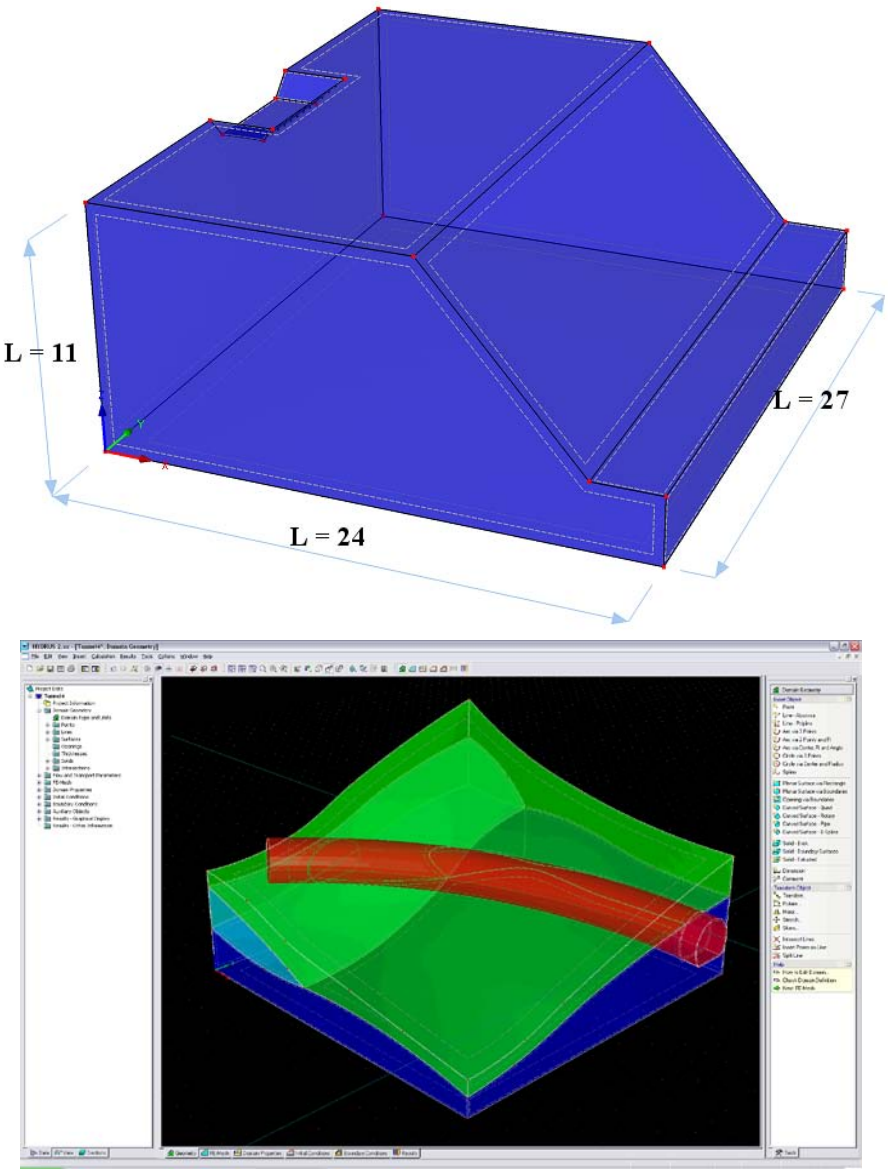


Figure 72. Examples of 3D-General Solids. Top - formed by Planar Surfaces, bottom – formed by Curved Surfaces.

General Solids can be created in the following ways:

1. Using a standard dialog, from which **Boundary Surfaces** can be picked graphically (individually, or using a **Quadrilateral** or **Rhomboid Selection Tool**).
2. Creating a **Simple Block** (**Brick**).
3. **Extruding** a **Solid** from a **Surface** (one or multiple simultaneously).

Process of Extruding:

Approach 1: Start a tool and click on a given **Surface**, which is to be extruded. It is important where a click occurs. The program finds a closest **Node** on a **Surface Boundary** and the extruding distance (height) is measured in this node. The extruding height is measured on a line passing through this node.

Approach 2: When you want to extrude multiple surfaces at the same time, you need to press the **Left Shift** keyboard button before selecting desired **Surfaces** (you can add or remove **Surfaces**). After a selection is made, release the Left Shift button and start extruding selected surfaces.

Approach 3: First select desired **Surfaces** and then click the **Edit Bar** command "**Solid – Extruded**". This will start the extruding process for all selected surfaces.

One can extrude **Surface** in the direction of *X*, *Y*, and *Z* axis, or in the direction perpendicular to an extruded **Surface**. When a **Surface** is not in a plane (e.g., is curved) and perpendicular extruding is selected, extruding is done in directions of local perpendicular lines to an extruded **Surface**.

During extruding one can select on the **Edit Bar** the length step (d*L*) or enter numerically desired length of extruding (*L*).

Note that the command **Extrude** can be used only for **Planar**, **Quad**, and **B-Spline Surfaces** and it cannot be used for **Partial Surfaces** and for **Surfaces** containing a zero **Curve** (i.e., a curve with a zero length from point P to point P).

4.5. *Thickness Vectors*

The term **Thickness Vector** is used for a vector (usually but not always perpendicular to the **Base Surface**) that extends the Base Surface to form a **solid** (the three-dimensional **computational domain**). A new **Thickness Vector** can be defined either graphically or numerically (Fig. 74).

There are several ways in which a **Thickness Vector** can be specified graphically and these are displayed at the **Edit Bar** (Fig. 73), which appears once a command for defining a **Thickness Vector** is selected.

a) **Point and Length:** A user specifies the length of the **Thickness Vector** on the **Edit Bar** (**Vector Length)** and with the mouse selects the point to which the Thickness vector is assigned.
b) **Point and Coordinate:** A user specifies the End Coordinate of the **Thickness vVctor** on the **Edit Bar** (**End Coordinate)** and with the mouse selects the point to which the Thickness vector is assigned. This method is suitable especially in case, when points located at the upper surface of the domain already exist (see Tutorial 2.07). In this case we need to specify **Thickness Vectors** whose upper points were read in from a GIS file and we need to create the lower (beginning) points that would be located in the plane of the **Base Surface**. Note (in the Tutorial) that the **Reverse Points** option was automatically checked on the **Edit Bar**. This is because the thickness Vectors have to originate from the **Base Surface** and not from the upper surface. If the **Reverse Points** option was not checked, Thickness Vectors would originate from the upper surface and end at the **Base Surface**.
c) **Two Points:** A user selects graphically two existing Points to form the **Thickness Vector**. In this case an **Anchoring** (beginning) **Point** of a **Thickness Vector** is the first selected point. It is therefore important to select points defining a **Thickness Vector** in the right order, i.e., to first select a point at the **Base Surface** and only then a point at the upper surface of the domain.
d) **Three Points:** A Thickness Vector is in general defined by three points: an **Anchoring Point**, a **Beginning Point**, and **an End Point** (Fig. 74). The **Anchoring Point** must be located in the **Base Surface**. The **Anchoring Point** is usually the same as the **Beginning Point** (i.e., both Point indices are the same) and one does not have to pay attention to it. However, in general, the **Anchoring Point** can be different than the **Beginning Point**, which leads to the so called “offset”. This option allows to define **Domains** that have both upper and lower surfaces deformed, i.e., not a plane.

Vector Direction can be specified to be a) Perpendicular to the Base Surface, b) in X-direction, c) in Y-direction, or d) in Z-direction.

Thickness Vectors can be defined by:
- clicking on individual Points
- selecting points with a rectangle (rhomboid, circle, polygon)
- clicking on a curve – Thickness Vectors will be added to all points of a curve.

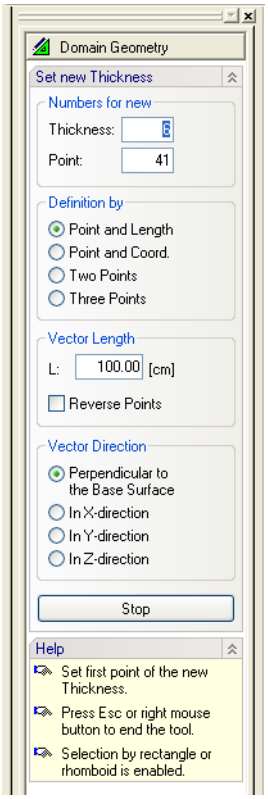


Figure 73. The Edit Bar during the process of graphically defining a Thickness Vector.

A definition of the **Thickness Vector** (i.e., its **Boundary Points**), is given and can be edited in the **Thickness** dialog window (Fig. 74).

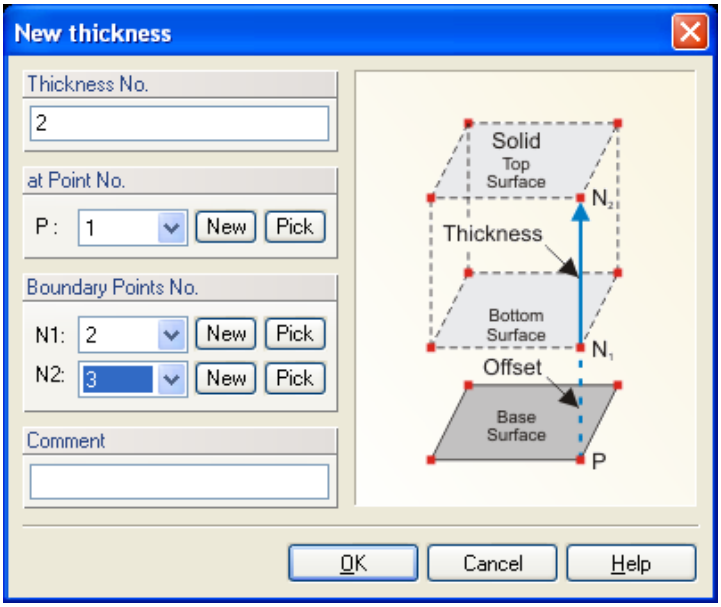


Figure 74. The Thickness dialog window.

The height of a solid is defined using one or more **Thickness vectors**. Each thickness vector is defined by an **Anchor Point P** and two **Boundary Points N1** and **N2**. The anchor point P must be part of the base surface, i.e., it must be either a defining point of the external boundary or the internal curve, or an internal point in the base surface. Boundary points N1 and N2 are arbitrary points in 3D space. Coordinates of these points can be edited, thus allowing one to specify the thickness vector in an arbitrary direction (i.e., not necessarily perpendicular to the base surface). Usually the anchor point P is the same as boundary point N1 so that one can use the same index for both P and N1. If, for whatever reason, we do not want to have the base surface on the bottom of the transport domain (Solid) (e.g., when the bottom of the transport domain is not in the same plane), users can make the N1 node be different from P (the red part in Fig. 75).

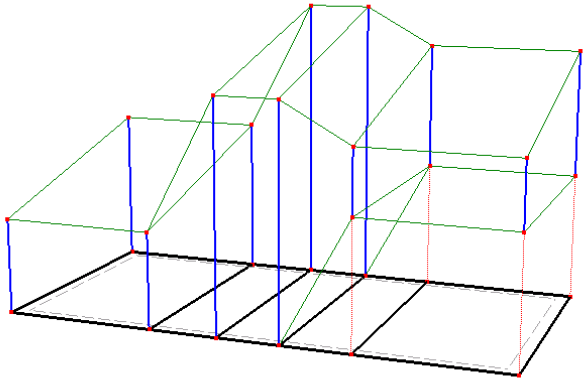


Figure 75. A solid with several thickness vectors.

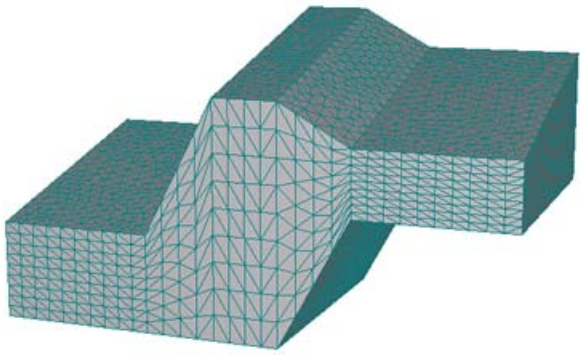


Figure 76. FE-Mesh for the solid in Figure 75.

The height of a solid is constant when less than three thickness vectors are used. Three thickness vectors define a linear plane (with generally an inclined surface). More than three thickness

vectors with different lengths then define the top surface that is formed by triangles, whose coordinates are calculated from the thickness vectors using linear interpolation or extrapolation.

When breaks in the slope of the top surface are to be defined exactly, then it is necessary to define internal curves in the base surface. Figures 77 and 78 show the importance of having internal curves (or not having them) in the Y direction for proper definition of the solid (compare Figures 75 and 77 Figures 76 and 78).

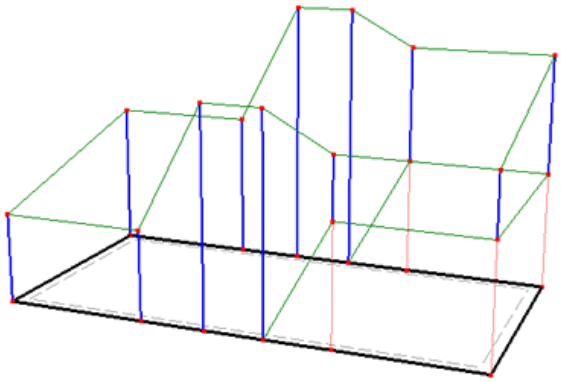


Figure 77. Missing internal curves in the base surface.

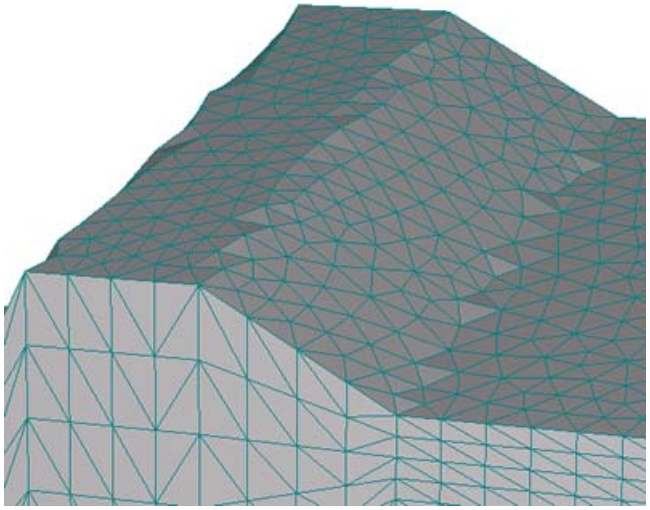


Figure 78. Consequence of missing an internal curve in the base surface on the FE-Mesh of the top surface.

Note: Three **Thickness Vectors** needs to be specified to define a **Domain** with a linearly changing thickness. As long as only two **Thickness Vectors** are specified, the thickness of the **Domain** is constant and defined using the first **Thickness Vector** (with lower index) (since three points are needed to define a plane).

4.6. Intersections of Surface and Solids

Intersections of Surfaces and Solids (Fig. 79) can be created using the following approaches:

A. **Intersection of Surfaces**: Select two or more **Surfaces**, click with the right mouse button on these selected **Surfaces**, and select the command "**Create Intersection**". When more types of different objects are selected (e.g., nodes, lines, or surfaces), which can, for example, occur when selection is made by a **Rectangle** (or a **Rhomboid**), then the command is located in the submenu "**Surfaces**".

B. **Intersection of Solids** (this option not yet available): Select two or more **Solids**, click with the right mouse button on these selected **Solids**, and select the command "**Create Intersection**". When more types of different objects are selected (e.g., nodes, lines, or surfaces), which can, for example, occur when selection is made by a **Rectangle** (or a **Rhomboid**), then the command is located in the submenu "**Solids**". For the **Intersection** „**Solids A-B**" (Fig. 79), the Solid A will remain in its original shape and the Solid B will be cut off. For the **Intersection** „**Solids B-A**", the Solid B will remain in its original shape and the Solid A will be cut off.

C. **Intersection of Surfaces and Solids** (this option not yet available): It is possible to create this intersection using the menu command *Insert->Domain Geometry->Intersection* or by clicking with the right mouse button on the item "**Intersections**" in the data tree of the **Navigator bar** and selecting "**Insert Intersections**" from the displayed popup menu. In the dialog, select desired type of Intersection (e.g., surfaces or solids).

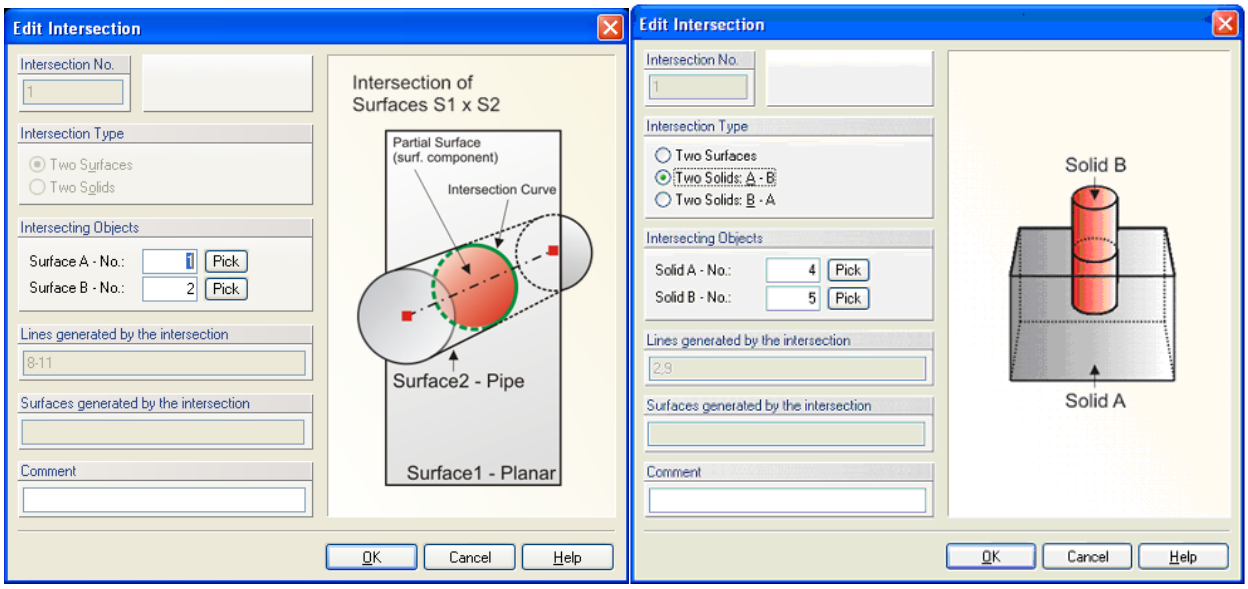


Figure 79. The Edit Intersection dialog window (for two Surfaces (left) and two Solids (right).

A **Partial** (or **Component**) **Surface** (Fig. 80) is created by an **Intersection of Surfaces** or **Solids**, which divides an original **Surface** into smaller **Sub-Surfaces**, or the so-called **Component Surfaces**. Although this **Surface** has its own number and can be used to define, for example, a **Solid**, its shape and boundaries are defined (generated) by the shape of its original **Surface** and a given **Intersection**. A list of **Components** resulting from division of the original **Surface** by an **Intersection** can be found on the **Tab Components**.

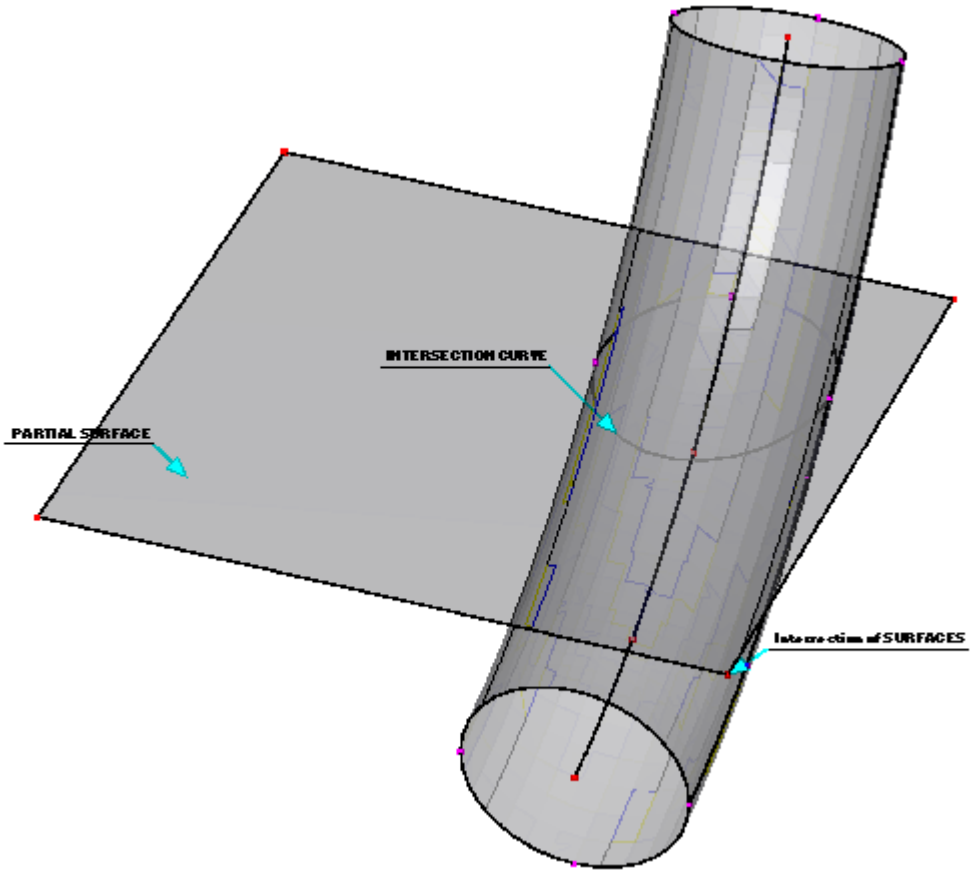


Figure 80. An example of an Intersection of two Surfaces and a resulting **Partial Surface** and **Intersection Curve**.

4.7. *Auxiliary Objects*

In addition to objects that define the computational domain, the HYDRUS GUI allows users to employ several **Auxiliary Objects** that can be used to, for example, add **Dimensions** to the computational domain, include various **Labels**, or define permanent **Cross Sections** or **Mesh-Lines**.

4.7.1. *Dimensions*

Dimensions can be added to describe spatial properties of the computational domain in the **View** window using the *Insert->Auxiliary Objects->Dimensions* command or the **Dimensions** command from the **Insert Object** part of the **Domain Geometry** version of the **Edit Bar**. Then one needs to click on two points defining the computational domain and drag **Dimensions** to the required position. Figure 98 shows an example of how **Dimensions** can be used.

After a command for defining a **Dimension** is selected, a user needs to first select by a cursor two existing points, the distance of which is to be labeled. The **Edit Bar** lists during this operation the two definition points and the Dimension number (Fig. 81 left). After the second point is selected, a cursor in the **View window** and the **Edit Bar** (Fig. 81 right) change and allow a user to define where a Dimension is to be displayed. In which plane a Dimension is to be displayed can be done on the **Edit Bar** (Fig. 81 right).

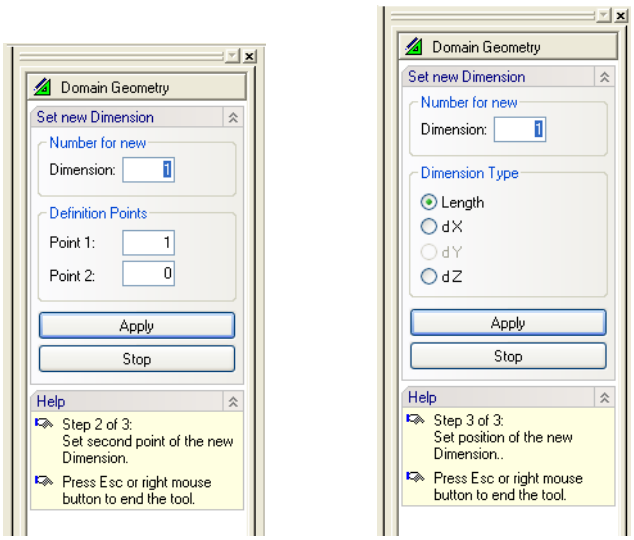


Figure 81. The Edit Bar during the process of graphically defining a Dimension. Selection of two definition points, the distance of which is to be labeled (left) and the dimension type (right).

4.7.2. *Labels*

Labels can add any desired text to the computational domain in the **View** window using the *Insert->Auxiliary Objects->Dimensions* command or the **Comments** command from the **Insert Object** part of the **Domain Geometry** version of the **Edit Bar**. One then clicks simply anywhere in the **View** window and write the desired text. The text itself, its color, frame, and its offset can be specified in the **Edit Comment** dialog window (Fig. 82). Figure 98 shows an example of how the "Furrow" **Label** is used.

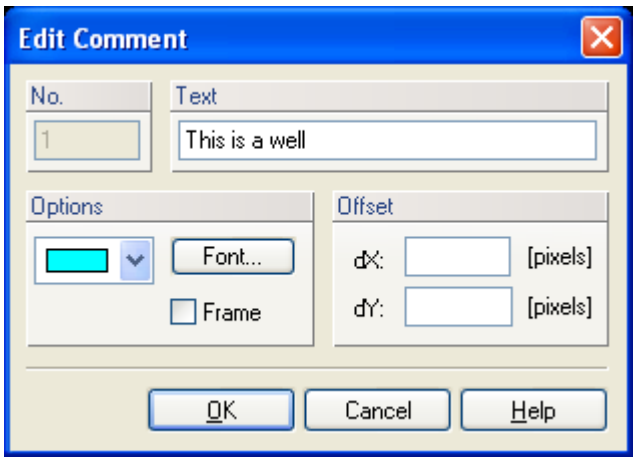


Figure 82. The Edit Comment dialog window.

After a command for defining a **Comment** is selected, a user needs to first select a location to which the comment will point using a cursor. The **Edit Bar** lists during this operation the coordinates of a cursor (**Position**), the color to be used for a comment, and the comment text (**Text**) (Fig. 83 left). A user can also select the **Font** to be used for the comment text.. After the position is selected, a user defines an **Offset** of the Comment text. The comment text, the comment font and color, and offset are displayed at the **Edit Bar** (Fig. 83 right).

4.7.3. *Bitmaps (Textures)*

Bitmaps (**Textures**) serve to use scanned figures (maps) as means to define the computational domain in the **View** window. **Bitmaps** can be added using the *Insert->Auxiliary Objects->Textures* command. Corners of the **Bitmap** must be anchored at 4 points, coordinates of which must be selected such that the scale of the Bitmap corresponds with the scale of the View window. Anchor points can be selected one at a time using either a Listbox (containing list of all defined nodes) or using a command **Pick** and selecting nodes using a cursor. All anchor points can be also selected simultaneously using a command **Pick ABCD**. The **Edit Bitmap** dialog window then provide information about the selected Bitmap, such as its **Size** in *pixels* and *kB*. One can then simply trace the bitmap to specify the computational domain.

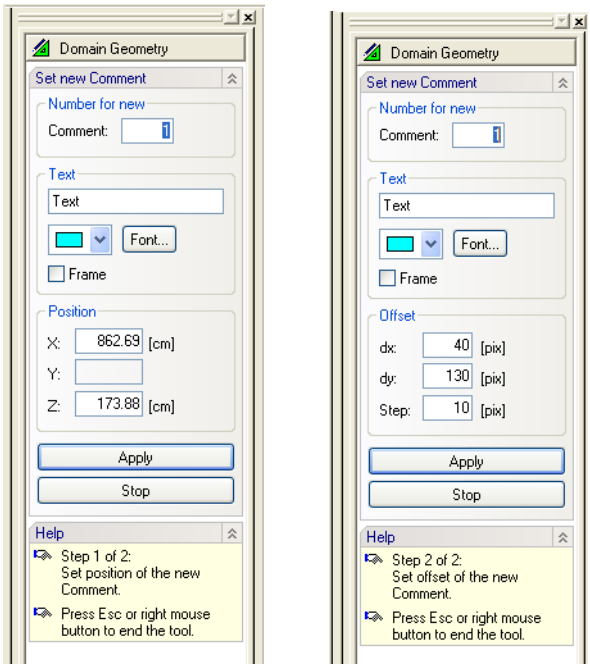


Figure 83. The Edit Bar during the process of graphically defining a Comment. Selection of the Comment Position, Comment Text, Font and Color (left) and Offset (right).

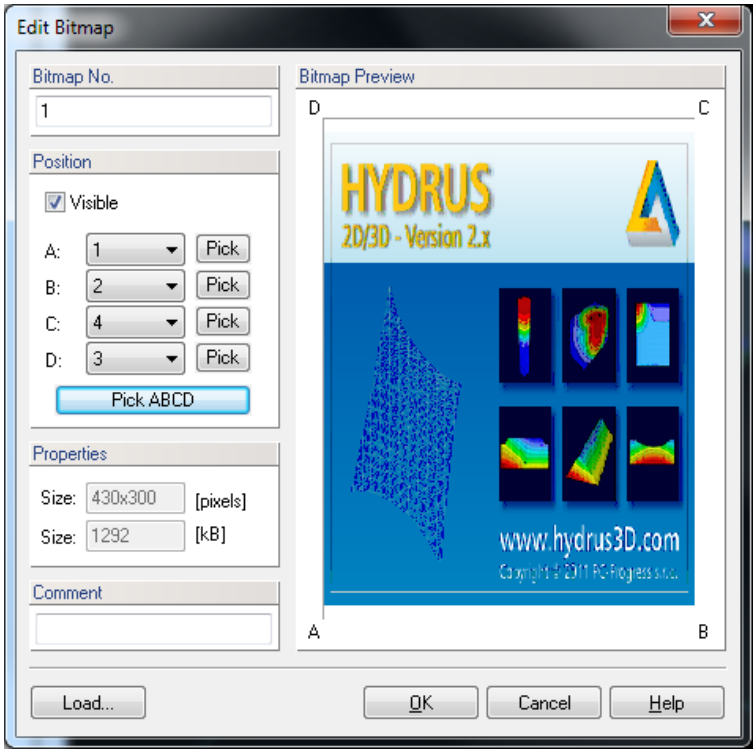


Figure 84. The Edit Bitmap dialog window.

4.7.4. *Cross-Sections*

In the HYDRUS-2D software package one could click at any two points of the transport domain to display results of selected variables between those two points, i.e., along a specified cross-section. The exact location of these cross-sections was not saved and they had to be redefined whenever a new graph was required. In HYDRUS one can define the cross-sections and save their locations so that graphs along the cross-sections can be recalled at any time by simply clicking at them. Graphs along pre-defined cross-sections can be display for both the initial conditions and the output results. For example, if a plot of the pressure head along a predefined cross-section at a particular time is needed, one needs to display the pressure head outputs, find a particular time, and then click on the predefined cross-section. The graph is displayed instantaneously. Specifying the cross-section within a two-dimensional domain is straightforward. For three-dimensional domains one can use the **Cross-Section** dialog window (Fig. 85) for this purpose.

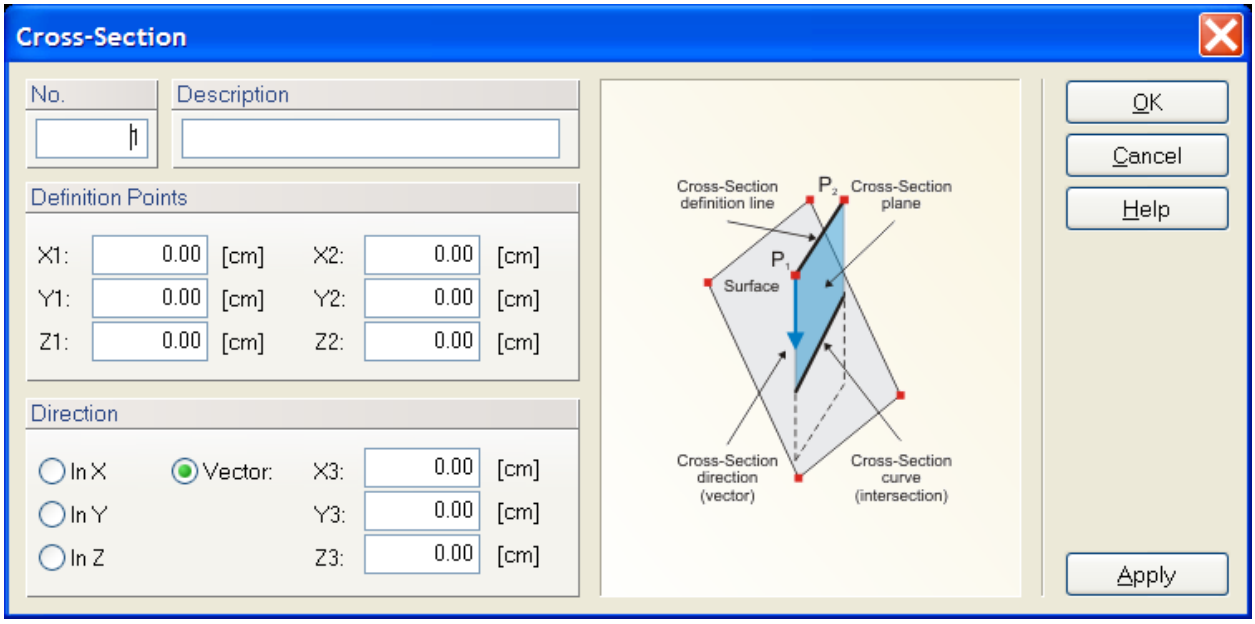


Figure 85. The Cross-Section dialog window.

4.7.5. *Mesh-Lines*

Mesh-Lines are very similar to **Cross-Sections**, except that **Mesh-Lines** follow edges of the finite elements and do not have to be straight. They are used, similarly to **Cross-Sections**, to display selected variables along defined **Mesh-Lines.** Similarly to **Cross-Sections**, the locations of **Mesh-Lines** are saved and can be recalled at any time.

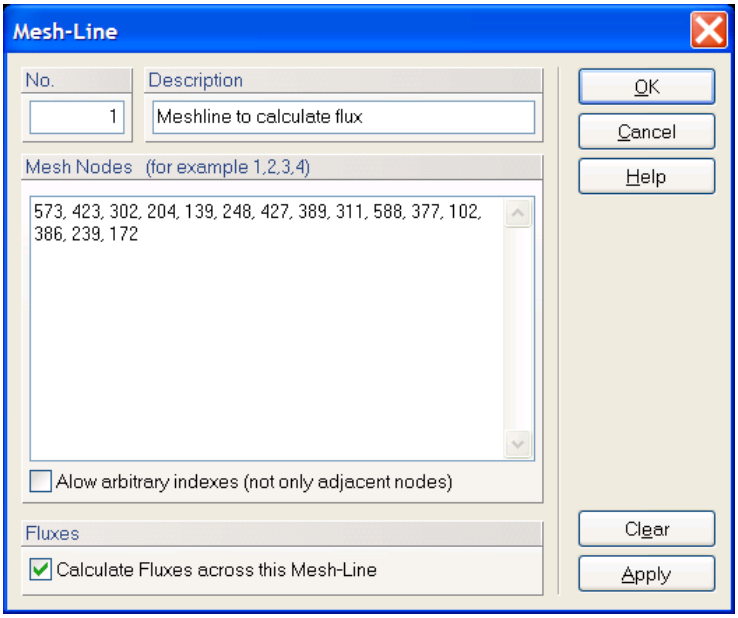


Figure 86. The Mesh-Line dialog window.

A description of the **Mesh-Line** is given in the **Mesh-Line** dialog window (Fig. 86), which contains the Mesh-Line number, its description, a list of nodes defining the Mesh-Line, and whether or not the computational module should calculate (actual and cumulative) water and solute fluxes across this Mesh-Line. The fluxes across the Mesh-Line are then displayed using the **Fluxes across Mesh-Lines** dialog window (Fig. 87) after using the *Results->Fluxes across Mesh-Lines* command. This dialog displays actual and cumulative, water and solute fluxes across individual **Mesh-Lines**.

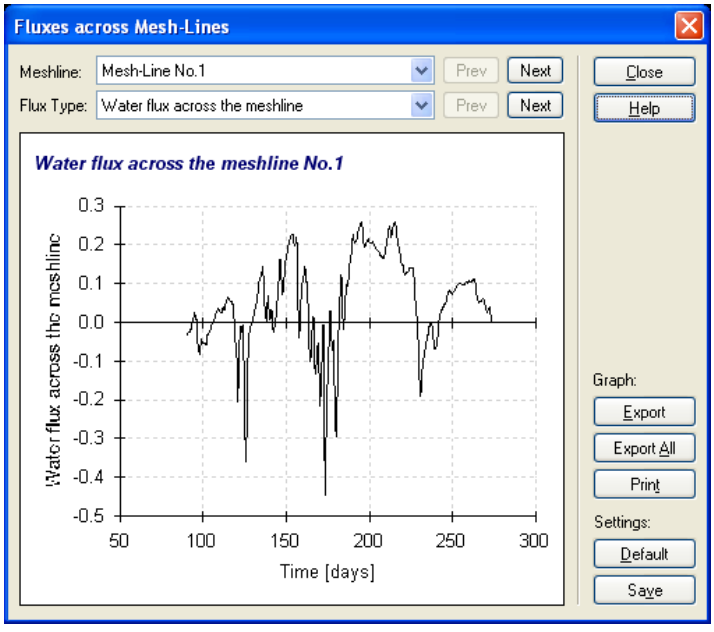


Figure 87. The Fluxes across Mesh-Line dialog window.

Information for this graph is read from the CrossSect.out file that contains data organized into the following columns:

Variable	Description	Units
Time	Time	[T]
Flux(i)	Water flux across the ith cross-section	$[L^2/T]$ or $[L^3/T]^{\dagger}$
CumFlux(i)	Cumulative water flux across the ith cross-section	$[L^2]$ or $[L^3]^{\dagger}$
SolFlux(i)	Solute flux across the i-th cross-section	$[M/L^3*L^2/T = M/L/T]$ or $[M/L^3*L^3/T = M/T]^{\dagger}$
CumSFlx(i)	Cumulative solute flux across the i-th cross-section	$[M/L^3*L^2 = M/L]$ or $[M/L^3*L^3 = M]^{\dagger}$

† for 2D and three-dimensional axisymmetrical problems, respectively.

4.7.6. *Background Layers*

Background Layers are geometrical objects that can serve as a template for defining the transport domain. A **Background Layer** consists of nodes and curves that are not part of the transport domain, but its components can be used to define the transport domain. A **Background Layer** is usually read from the DXF file (AutoCAD) (Figure 89). An example of a very complex Background Layer (unrelated to hydrology) read from the DXF file is given in Figure 88.

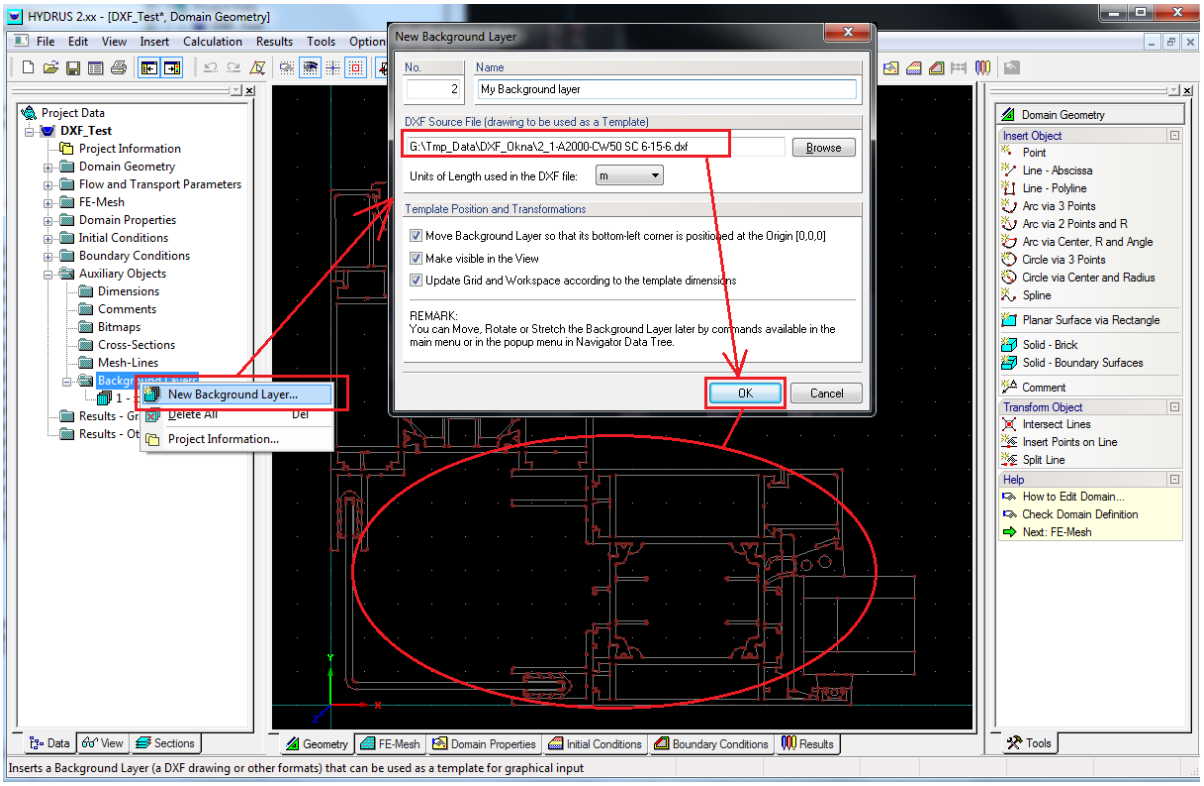


Figure 88. An example of the Background Layer.

The project may have at the same time multiple **Background Layers** (virtually any number) and their visibility can be turned on and off using the View Tab at the Navigator Bar (*Auxiliary Objects->Background Layers*). **Background Layers** are displayed in the View window using suppressed (less intense) colors, so that they do not visually disturb when objects of the geometry are being defined. The intensity of display and other parameters can be set (intensity of their display can be set between 0 and 1) in the **Display Options** dialog window (the Menu command *Options->Display Options->Edit*) (Fig. 126). If the location of the template (background layer) is not satisfactory, it can be **Moved** (Fig. 52), **Rotated** (Fig. 53, left), **Mirrored** (Fig. 53, right), **Stretched** (Fig. 54, left), and/or **Skewed** (Fig. 54, right) as needed.

4.8. *Other Notes on Objects*

Objects **Mesh Refinement** define a local density of the FE-Mesh in the vicinity of a particular object. Possible types of Mesh Refinement are:

- Mesh Refinement at Point
- Mesh Refinement on Curve given by number of points
- Mesh Refinement on Curve given by FE size
- Mesh Refinement on Surface

4.8.1. *Object Numbering*

Each object has its own number (index) that serves for unique identification of an object for operations such as Edit, Delete, or Find. Object numbering is fully controlled by the user (a user specifies the object index) and does not have to be continuous (indexes do not have to sequentially increase).

4.8.2. *Relations among Objects*

More complex objects are defined using simpler objects. For example, a surface is defined by indices of its boundary curves, and a boundary curve is defined by indices of its points. The curve, however, does not own its points, since these points can also be used to define other curves. This is especially true for points at the beginning and end of a curve, since these points are usually used also by neighboring curves. A relation „Parent – Descendent“ exists among objects. In case of a curve, points are „Parent“ objects and a Surface is its „Descendent“.

4.8.3. *References among Objects and Convention for Writing a List of Indices*

Objects are referenced using a list of indices. A list of indices is written using a text format, where individual indices are separated by a comma and dash (-) between two indices indicates a range “from – to” (e.g., 1,5-10,35-30,8,11). After inserting new indices, the list is always reformatted to minimize the length of the text. Depending on circumstances, the list of indices respects/does not respect sequence, in which objects were defined.

4.9. *Import Geometry from a Text File*

It is possible to **Import** definition of objects defining the **Geometry** of the transport domain from a text file using a command “*Import Geometry from a Text File*”. It is possible to import (export) points, curves (polylines, circles, arcs, and splines), surfaces, openings and thickness vectors.

a) Definition of each object starts with the word **OBJECT=KEY_WORD**, followed by coordinates of points defining given object. Two or three coordinates (for two- and three-dimensional problems) of a single point are given on a single line. Numbers can be delimited using a space, a semicolon, or a tabulator.

b) Points associated with higher objects, i.e., lines, openings or surfaces, are listed as part of this object. Similarly, lines associated with higher objects, i.e., openings or surfaces, are listed as part of this object. Only points that are not part of any higher object should thus be listed under the object POINTS, and only lines that are not part of any higher object (e.g., that do not form boundaries of surfaces) should thus be listed under the object LINES.

c) Lines with a semicolon at the beginning are ignored as „Comments".

d) It is possible that exported Geometry once imported back into HYDRUS can have different numbering, i.e., the project may not be identical.

e) Below is a list (**KEY_WORD**) of all possible objects. "**POLYLINE**" is a single line defined by multiple nodes, while "**LINES**" is a series of lines (multiple objects). **Surfaces** or **Openings** must be defined by a single closed curve, the type of which is given in the name of the object (e.g. SURFACE_CIRCLE). When this rule is not fulfilled (e.g., for a surface with complex boundary), this complex boundary will be saved as a series of lines, i.e., SURFACE_LINES.

f) The **THICKNESS_ARR3Z_NLAYERS** command allows importing multiple **Thickness Vectors** to define variable thickness of a **Solid**. On each Thickness Vector one can define multiple z-coordinates that are used to divide a Solid automatically into Layers with variable thicknesses. The number of Layers is arbitrary (min=1, max=100) and their number is given by the number of columns in the file.

KEY_WORD for Import/Export:

```
POINTS
LINES
POLYLINE
SPLINE
CIRCLE
ARC
SURFACE_LINES
SURFACE_POLYLINE
SURFACE_SPLINE
SURFACE_CIRCLE
OPENING_LINES
OPENING_POLYLINE
OPENING_SPLINE
OPENING_CIRCLE
THICKNESS
THICKNESS_ARR3Z
THICKNESS_ARR3Z_NLAYERS
```

Notes on the **THICKNESS_ARR3Z_NLAYERS** command (the **THICKNESS_ARR3Z** command has only the first five columns):

Particular columns in the input file have the following meaning:

1. X coordinate.
2. Y coordinate.
3. Z coordinate of the Definition Point of the Thickness Vector (Anchor Point, see Figure 74 of the User Manual with the Edit Thickness Vector dialog and the point denoted "P"). The Definition (Anchor) Point must lie in the plane of the Base surface. The Z-coordinate in the third column will thus likely be constant for all Thickness Vectors, unless the Base Surface is inclined.
4. Z coordinate of the lower point of the first layer of the Thickness Vector (a point denoted "N1" in Figure 74 of the User Manual). When P=N1, this coordinates is the same as the 3rd coordinate.
5. Z coordinate of the upper point of the first layer of the Thickness Vector.
6. Z coordinate of the upper point of the second layer of the Thickness Vector.
7. …
8. Z coordinate of the upper point of the last layer of the Thickness Vector, i.e., the coordinate of the surface of the solid.

Here is an example of the file for the import of a Solid divided into three Geo-Layers:

```
OBJECT=THICKNESS_ARR3Z_NLAYERS
  4.500000e+000   4.000000e+000   0.000000e+000   0.000000e+000   1.300000e+000   2.100000e+000   3.300000e+000
  5.500000e+000   2.500000e+000   0.000000e+000   0.000000e+000   1.300000e+000   2.200000e+000   3.400000e+000
  7.000000e+000   4.500000e+000   0.000000e+000   0.000000e+000   1.400000e+000   2.300000e+000   3.000000e+000
  7.000000e+000   2.500000e+000   0.000000e+000   0.000000e+000   1.200000e+000   2.600000e+000   3.500000e+000
  6.500000e+000   9.999999e-001   0.000000e+000   0.000000e+000   1.600000e+000   2.400000e+000   3.600000e+000
  5.000000e+000   2.000000e+000   0.000000e+000   0.000000e+000   1.200000e+000   2.500000e+000   3.700000e+000
  4.500000e+000   2.000000e+000   0.000000e+000   0.000000e+000   1.400000e+000   2.400000e+000   3.400000e+000
  5.000000e+000   9.999999e-001   0.000000e+000   0.000000e+000   1.500000e+000   2.500000e+000   3.300000e+000
  5.500000e+000   9.999999e-001   0.000000e+000   0.000000e+000   1.100000e+000   2.100000e+000   3.200000e+000
;
```

Other notes:

9. The minimum number of columns is 5 (this corresponds to a single layer).
10. Z coordinates must be entered in the correct sequence, i.e., from the bottom (Base Surface) up towards the end of the Thickness Vector.
11. If layers are to be defined in a different direction than Z (e.g., when the Base Surface lie in the XZ plane), one needs to first carry out the standard import in the Z direction and then to rotate the entire domain using the Rotate function.
12. When the "THICKNESS_ARR3Z_NLAYERS" is used, i.e., the input file includes data of thickness vectors with multiple geo-layers, this key word can be processed fully only if the domain already contains a 3D-Layered Solid. If there is no Solid defined yet, then HYDRUS is not able to create a Solid automatically from imported points because its Base Surface can have a very complex shape. There are two ways how to proceed:
    a) Press "OK" to continue. HYDRUS will import first only thickness vectors without geo-layers. Then define a 3D-Layered Solid using imported points and import the same file again. Geo-layers will be added to the Solid during this second import.
    b) Press "Cancel" to cancel this import. First define a 3D-Layered Solid and then import this file again. Thickness vectors with layers will be added to the Solid.

4.10. *Import Geometry from a DXF File*

It is possible to **Import** the definition of objects defining the **Geometry** of the transport domain from a file in the DXF format. **AutoCAD DXF** (Drawing Interchange Format, or Drawing Exchange Format) is a CAD data file format developed by Autodesk for enabling data interoperability between AutoCAD and other programs. Autodesk now publishes the *DXF specifications* on its website for versions of DXF dating from AutoCAD Release 13 to AutoCAD 2010. The menu command **Import Geometry from a DXF File** calls the dialog window (Fig. 89) of the same name that allows users to select (or browse for) the DXF file with the description of the transport domain, and to specify units that are used in this file.

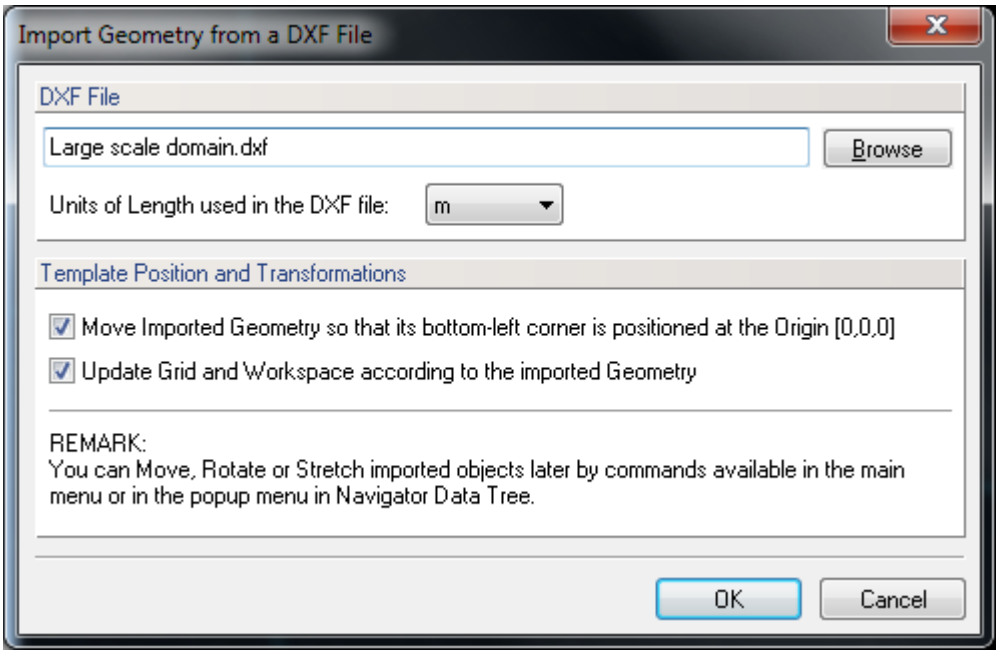

Import Geometry from a DXF File
DXF File
Large scale domain.dxf
Browse
Units of Length used in the DXF file:
m
Template Position and Transformations
Move Imported Geometry so that its bottom-left corner is positioned at the Origin [0,0,0]
Update Grid and Workspace according to the imported Geometry
REMARK:
You can Move, Rotate or Stretch imported objects later by commands available in the main menu or in the popup menu in Navigator Data Tree.
OK
Cancel

Figure 89. The Import Geometry from a DXF File dialog window.

Since local coordinates defining the transport domain in the coordinate system used in the DXF files may include very large numbers, users can ask the HYDRUS GUI to convert these coordinates so that the bottom-left corner of the transport domain is located in the origin of the computational coordinate system. This will likely lead to much smaller values of local coordinates. Finally, users can ask the HYDRUS GUI to automatically adjust the Grid and Workspace variables to accommodate the imported geometry.

4.11. *Import Geometry from a TIN File*

It is possible to also Import the definition of objects defining the Geometry of the transport domain from a file in the TIN format. TIN files are used for storing triangulated irregular networks using a simple set of xyz coordinates. The TIN file specifications are at:
http://www.ems-i.com/wmshelp/Files/File_Formats/TIN_Files.htm.

5. Finite Element Mesh

5.1. *Finite Element Mesh Generator*

The **Finite Element Mesh Generator** dialog window was used in earlier versions to select a structured finite element mesh for relatively simple rectangular or hexahedral domain, or a more general unstructured finite element mesh. The dialog provided a brief description of each mesh generator and a simple bitmap with an explanation of the main terms involved. In later versions (after 1.03) a decision which generator to use is made in the Domain Type and Units Window (Fig. 6 and 7). While the structured finite element generator can be used only for simple rectangular (i.e., the Geometry Type "2D-Simple (Parametric)" - see the Projects Geometry Information Section 2) or hexahedral domains (3D-Simple (Parametric)), the unstructured finite element generator is used for more complicated geometries (i.e., 2D-General (Boundary Rep.), 3D-Layered, and 3D-General (Boundary Rep.)). While the unstructured mesh generator **MeshGen2D** is used to generate FE meshes for two-dimensional domains (2D-General (Boundary Rep.)) and for the **Base Surface** of three-dimensional layered domains (3D-Layered), the mesh generator **Genex/T3D** is used to generate three-dimensional FE meshes for the 3D-General (Boundary Rep.) geometry.

5.2. *Structured Finite Element Mesh Generator*

As discussed in Section 2, two-dimensional transport domains can be defined using modified rectangles. Simple rectangular domains are defined by three straight lines, one at the bottom of the domain and two at the sides, while the upper boundary may or may not be straight (see examples in Fig. 8). Nodes along the upper boundary may in that case have variable *x*- and *z*-coordinates, but the lower boundary line must be straight (horizontal or with a specified slope), whereas the left and right boundary lines must be vertical. The flow region can then be discretized into either a structured or an unstructured triangular finite element mesh.

When the structured mesh is used one then needs to specify in the **Rectangular Domain Discretization** dialog window the number of nodes (*Count*) on the horizontal (*Horizontal Discretization in X-Direction*) and vertical (*Vertical Discretization in Z-Direction*) sides of the rectangular region, including their nodal coordinates (Fig. 90). The *relative size of finite elements* on the vertical side can be modified using the RS1 (relative size at the top) and RS2 (relative size at the bottom) factors below *General Vertical Coordinates*. The element sizes are then proportionally distributed. Smaller RS factor leads to smaller elements.

The upper boundary is by default parallel with the bottom boundary. Any possible vertical deviations from this parallel line can be defined using *dz* values (in the *Horizontal Discretization in X-Direction* part of the window). Relatively general domains can still be defined by properly adjusting the *dz* values (see Fig. 8).

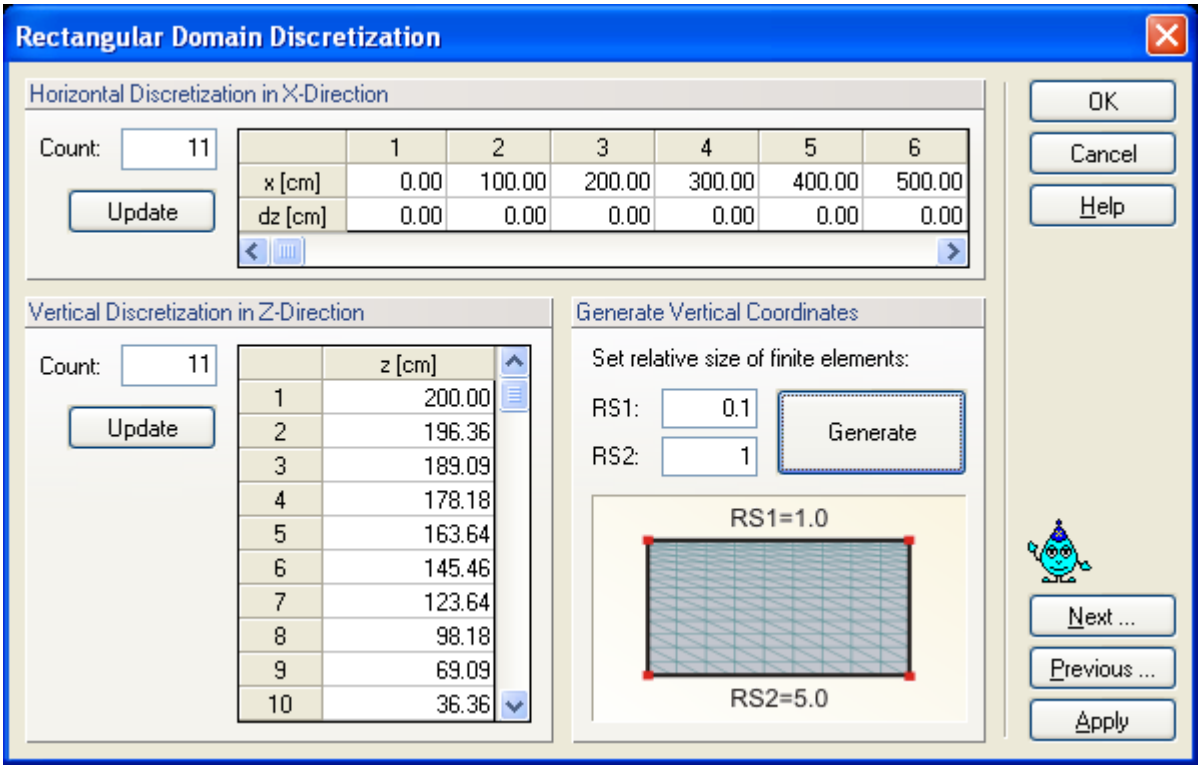


Figure 90. The Rectangular Domain Discretization dialog window.

A similar approach can be used to discretize simple hexahedral domains in three dimensions. Hexahedral domains must have similar properties as rectangular domains in that they are defined by vertical planes at the sides, a horizontal plane (possibly with a certain slope) at the bottom boundary, and with only the upper boundary not having to be a plane. The discretization of the hexahedral domain is then defined in the **Hexahedral Domain Discretization** dialog window. Again, one needs to specify the number of nodes (*Count*) on the horizontal (*Horizontal Discretization in X*, *Horizontal Discretization in Y*) and vertical (*Vertical Discretization in Z-Direction*) sides of the hexahedral region and their nodal coordinates (Fig. 91). The *relative size of finite elements* on the vertical side can again be modified using RS1 (relative size at the top) and RS2 (relative size at the bottom) factors (*General Vertical Coordinates*). The vertical final element sizes are then proportionally distributed.

Any possible vertical deviations from the plane parallel with the bottom of the domain can be defined using the *dz* values (in the *Horizontal Discretization in X* and *Horizontal Discretization in Y* parts of the window). This feature still allows relatively general domains too be created (see Fig. 9).

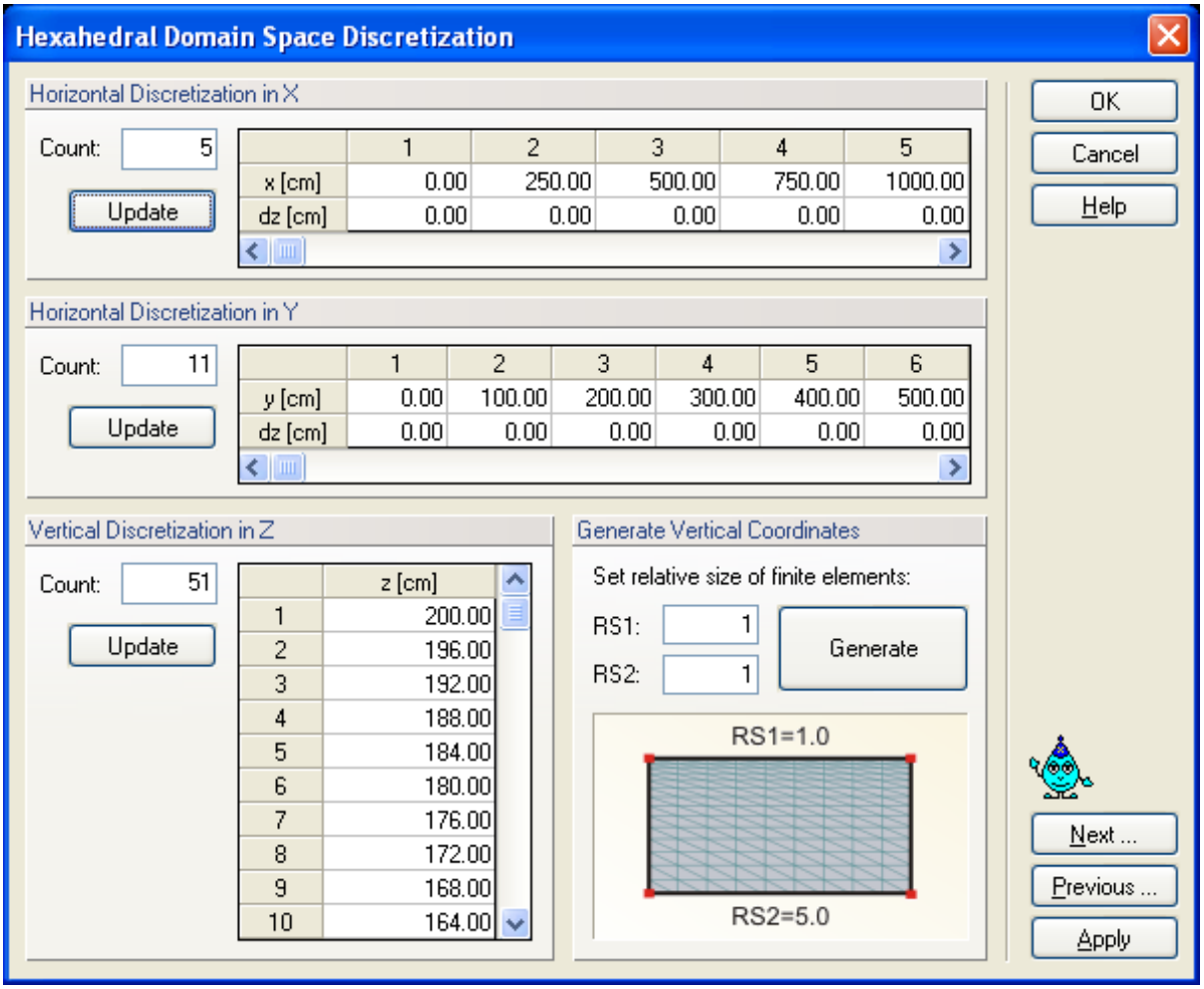


Figure 91. The Hexahedral Domain Discretization dialog window.

5.3. *Unstructured Finite Element Mesh Parameters*

Parameters for generating the *Unstructured Finite Element Mesh* are specified in the **FE-Mesh Parameters** dialog window (Figs. 92 through 95). This dialog window has six and four Tabs for the MeshGen2D and T3D generators, respectively, in which various parameters of the unstructured finite element mesh can be specified.

The Main Tab

The *Targeted FE size* (i.e., the average size of the triangular elements in the generated finite element mesh) is specified on the **Main** Tab (Figs. 92). The program selects by default a **Targeted FE Size**. Users can change this value by deselecting the **Automatic** check box. The finite element mesh with this *Targeted FE size* can be further modified using various tools, such as *Stretching* in different directions (on the **Stretching** Tab, Fig. 93) to make the mesh anisotropic, specifying the *Maximum Number of Nodes on Boundary Curve* (on the **MG-Options** Tab, Fig. 94) and *Minimum Number of Nodes on Boundary Curve* (on the **Options** Tab, Fig. 95), and using **Finite Element Mesh Refinement** (Fig. 97). While the **Default** command sets default values on a particular tab of the **FE-Mesh Parameters**, the **All Default** command sets default values on all four tabs. For three-dimensional applications (only for 3D-Layered geometries), a user can specify on the **Main** Tab the **No. of Horizontal Layers**, which are layers parallel with the **Base Surface** to add the third dimension to the problem and if the finite elements used to discretize the three-dimensional domain are to be **Tetrahedrals** or **Triangular Prisms** for 3D-Layered geometries, or **Tetrahedrals** or **Mixed Elements** (multiple types of elements) for 3D-General geometries. It is recommended to use Triangular Prisms or Mixed Elements rather than Tetrahedrals since then the number of finite elements is three or more times smaller and thus the calculations are faster.

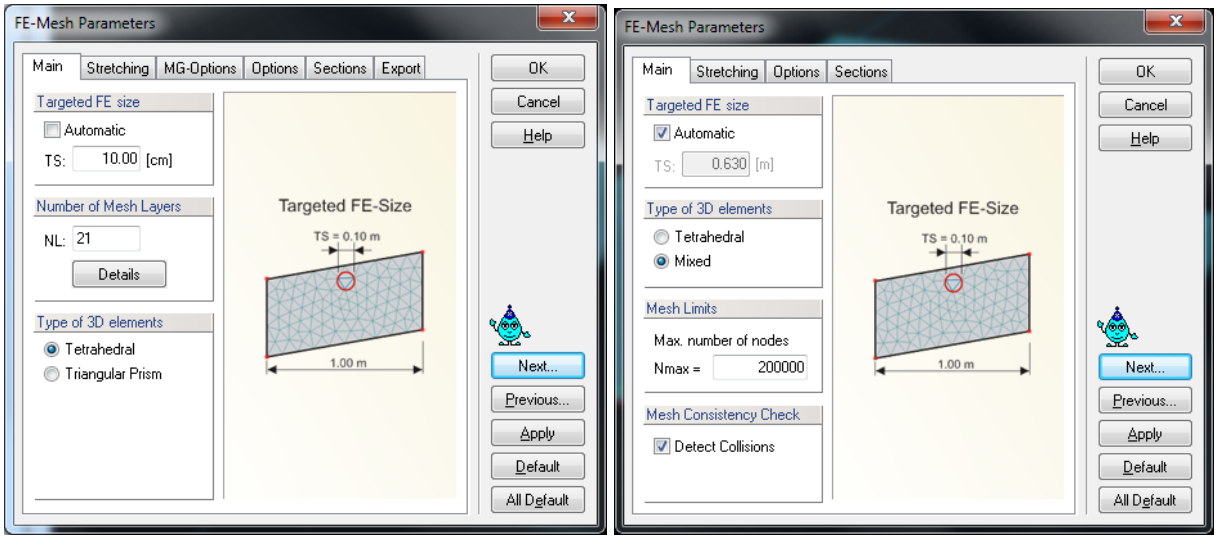


Figure 92. The FE-Mesh Parameters dialog window (the Main Tab for 3D-Layered (left) and 3D-General (right) geometries).

For 3D-General geometries, users also need to specify the **Maximum Number of Nodes** in the FE mesh. This is the maximum number of finite element nodes in the entire three-dimensional domain. Similarly as below for MeshGen when this is specified for a two-dimensional domain (Fig. 94) when this maximum number is reached a warning will appear ***Achieved the maximum number of nodes!*** This means that the maximum allowed number of nodes was reached during the mesh generation process and the user needs to decide whether or not so many nodes are needed for the envisioned FE mesh and either increase this number or adjust other parameters so that less nodes (and FE elements) are generated.

For 3D-General geometries, there is in the **Mesh Consistency Check** section an additional check box **Detect Collisions**. This check box is important only for complex 3D-General geometries consisting of multiple solids. When this check box is on, the program checks "**collisions**" of different objects. The solids cannot intersect each other without having the intersections properly defined using boundary curves. The program also detects if one **Solid** is entirely inside of another Solid (i.e., its boundaries do not intersect). The former Solid has to be in such case defined as an **Opening** (Hole, **Cavity**). The check box "Detect Collisions" enables users to turn off this check in cases, when they are absolutely sure that there are no such collisions and they still receive warning about a collision of solids.

The Stretching Tab

Stretching of the finite element mesh (i.e., the degree of mesh anisotropy in a certain direction) is defined using the **Stretching Factor** and **Stretching Direction** (Fig. 93). The finite elements are made larger in the particular **Stretching Direction** if the **Stretching Number** is larger than one, and smaller if smaller that one. The result of this transformation is a mesh deformed in the given direction, which can be desirable for problems that, for example, require different spatial steps (mesh sizes) in the *X* and *Y* directions. The **Stretching Direction** is defined by a vector with two coordinates (*Vx* and *Vz*) for vertical two-dimensional domains. For three-dimensional problems this vector requires three components (*Vx*, *Vy*, and *Vz*). An example of a mesh stretched using a **Stretching Factor** of 3 in the *x*-direction is shown in Figure 103.

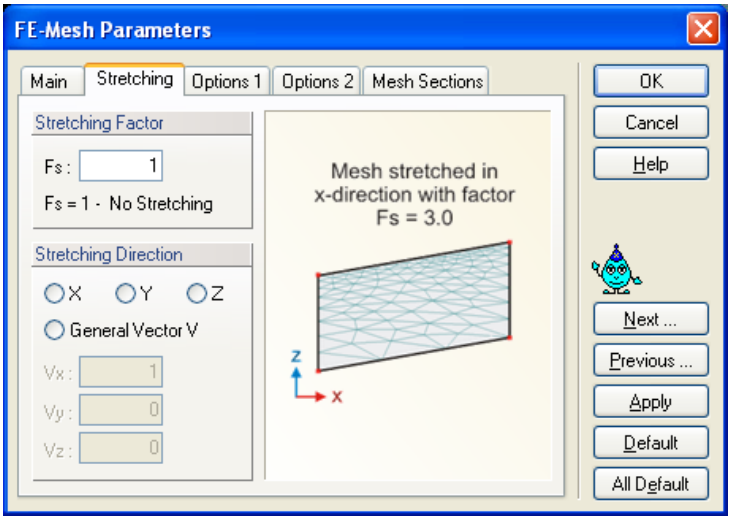


Figure 93. The FE-Mesh Parameters dialog window (Tab Stretching).

The MG-Options Tab

Parameters for the unstructured triangular finite element generator are given in the **MG-Options** (Meshgen) Tab of the **FE-Mesh Parameters** dialog window (Fig. 94). The parameters are divided into *FE-Mesh Limits* (which limits the number of elements) and *FE-Mesh Quality* (which affects the smoothness of the FE mesh) groups.

The following parameters are specified in the ***FE-Mesh Limits*** group:

Maximum Number of Nodes on Boundary Curves: This is the maximum total number of nodes on all boundary curves for two-dimensional applications, or on all boundary curves defining the bottom plane (base surface) for three-dimensional applications.

Maximum Number of FE-Mesh Nodes (2D Mesh): This is the maximum total number of finite element nodes in two-dimensional domains, or on the bottom plane (base surface) of three-dimensional domains.

Both parameters are mainly informative and may lead to an interruption of the FE-mesh generation process. The mesh generation is interrupted by the message**: *Achieved the maximum number of nodes!*** This means that the maximum allowed number of nodes (either on the boundary curves or in the two-dimensional domain) was reached during the mesh generation process. This is usually a consequence of having too many nodes along the boundaries (the number of mesh nodes inside a domain increases approximately with the square of the number of boundary nodes). It is then necessary to decide whether or not so many nodes are needed for the envisioned triangular mesh. If the answer is 'yes' then the maximum number of nodes must be increased in this dialog window. If the answer is 'no' then it is necessary to decrease the **Targeted FE Size** (Figs. 92) or to increase the **Smoothing Factor** (in the *FE-Mesh Quality* group discussed below).

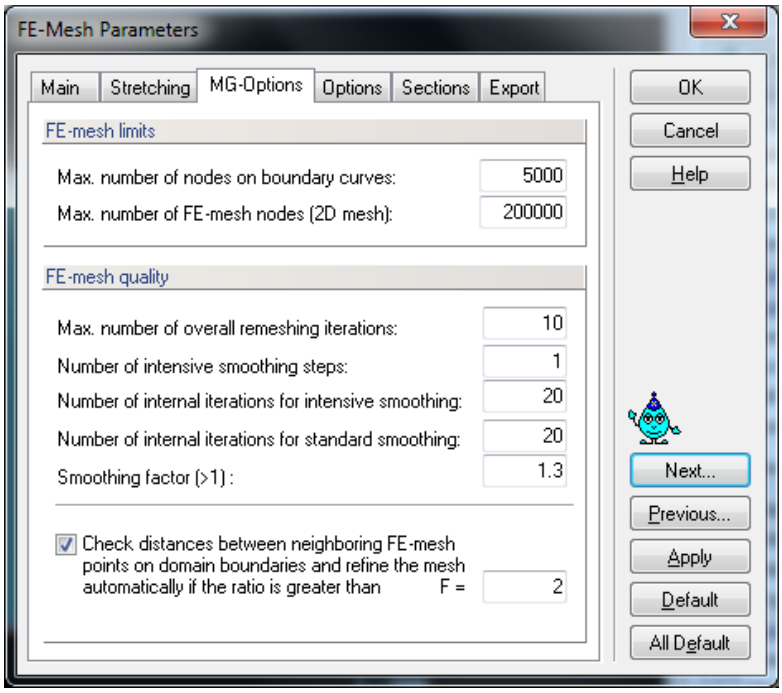


Figure 94. The FE-Mesh Parameters dialog window (Tab MG-Options).

The following parameters are specified in the ***FE-Mesh Quality*** group:

Maximum Number of Overall Remeshing Iterations:
This number defines the maximum number of iterations during finite element mesh remeshing. In most cases the resulting mesh is obtained within fewer iterations than the default value of 10. In some cases the repeated adding and removing of nodes can cause an infinite loop. In that case (or when the mesh generation process converges very slowly) the code terminates after reaching the maximum number of iterations as defined by this value.

Number of Intensive Smoothing Steps:
Intensive smoothing repeats the operations of Delaunay remeshing and smoothing until there are no more changes during the Delaunay remeshing step. This parameter specifies the number of intensive smoothing cycles in the beginning of the mesh generation process, which can significantly influence the mesh smoothness. However, too many smoothing cycles can significantly slow down the mesh generation process. The recommended value is between 1 (less smoothing) and 3 (more smoothing).

Number of Internal Iterations for Intensive Smoothing:
This number defines the maximum number of iterations during one intensive smoothing step. This number guaranties that intensive smoothing will stop after a specified number of iterations, even when the prescribed criterion is not reached (i.e., some changes would still occur during Delaunay remeshing).

Number of Internal Iterations for Standard Smoothing:
This number defines the maximum number of iterations while solving the elliptic equations, a process needed during mesh smoothing; it significantly influences the final smoothness of the mesh. A higher number of iterations improves the mesh smoothness. It serves little purpose to increase the number above 20 since the mesh is then virtually constant anyway, while the whole process of mesh generation would be slowed down significantly.

Smoothing Factor:
The smoothing factor is the ratio of the maximum and minimum height of a finite element triangle. For a triangle with equal sizes this factor is equal to 1 (which is theoretically not achievable for finite element meshes). The smoothing factor can be decreased to a value of about 1.1 when a highly smooth finite element mesh is required and, vice-versa, can be increased when a course mesh can be tolerated. The smoothing factor significantly affects the final number of elements.

In general, the default values in the FE-Mesh Parameters dialog window should be preserved; only experienced users should modify the various parameters needed for the mesh generation process.

The Options Tab

Minimum Number of Points Boundary Curves is set by default equal to 15. This number can be changed in the **FE-Mesh Parameters** dialog window of the **Options** Tab (Fig. 95). This parameter is important when such objects as openings representing wells or drains are included in the transport domain. These objects may be very small compared to the global finite element mesh (i.e., smaller than the targeted finite element size). Having a minimum number of nodes on boundary curves will then lead to local refinement of the finite element mesh around these objects, thereby ensuring that relatively small objects are accurately represented in the numerical solution.

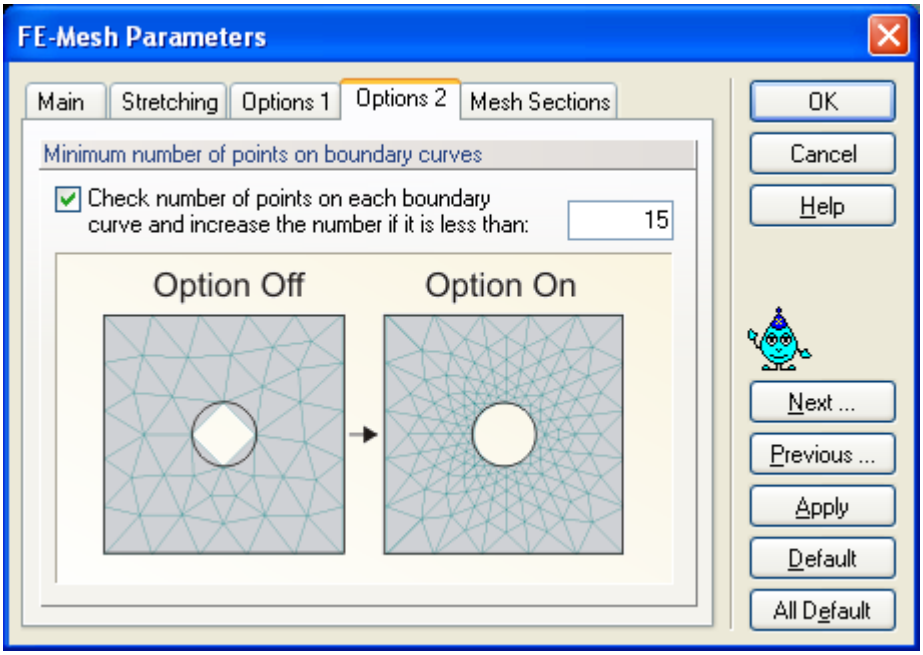


Figure 95. The FE-Mesh Parameters dialog window (Tab Options).

The Export Tab

In the **Export Tab** (not shown), users can select options for export of the FE-Mesh to a text file. One can, for example choose, which points to export (including or excluding the intermediate points on boundary curves) and whether or not to include in the export also internal curves.

The Mesh Section Tab

The program can generate default **FE-Mesh Sections** (the **Mesh Section** Tab of the **FE-Mesh Parameters** dialog window, Fig. 96) or FE-Mesh Sections (for detailed description, see Section 5.7) can be created by a user. Default FE-Mesh Sections depend on the geometry of the transport domain. For examples, default section include: a) Entire FE Mesh, b) Vertical (horizontal) shell, and c) Each horizontal (vertical) layer. Mesh Sections can also be generated for each **Geo-Section** (see Section 8.1.8). The **Mesh Sections** are generated automatically when the FE-Mesh is generated or anytime using the menu command *Edit->Sections->Generate Sections* (note that the dialog window to **Options for Generation of Geo-Sections and FE-Mesh Sections** (Fig. 139) is similar to the **Sections** Tab of the **FE-Mesh Parameters** window (Fig. 96)).

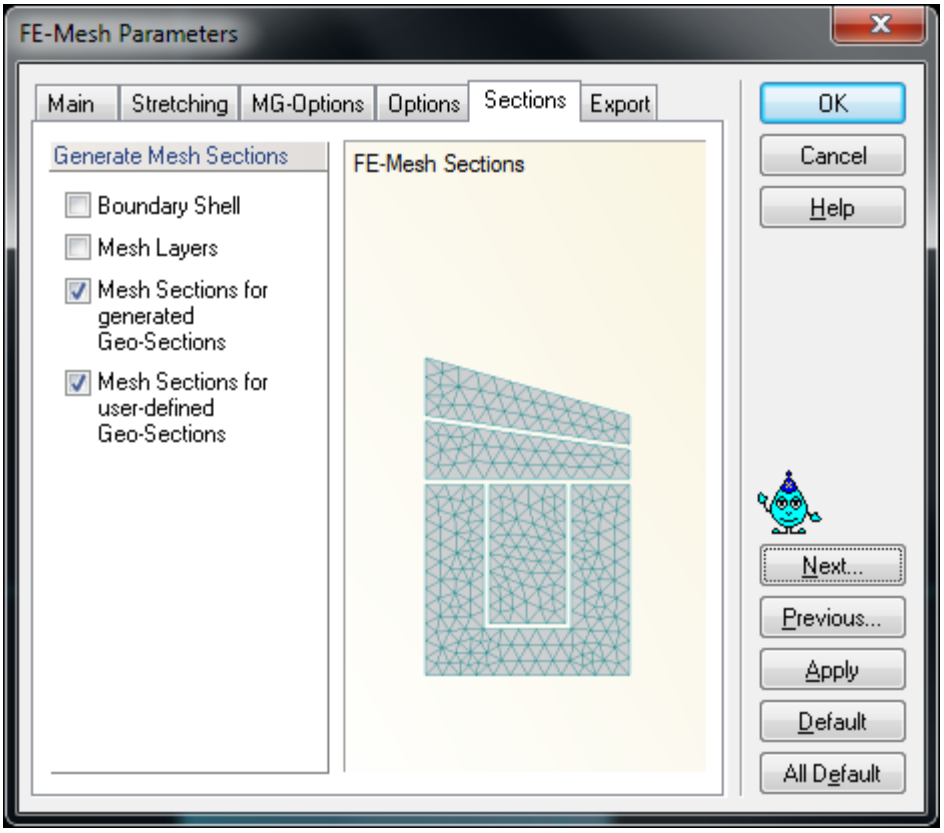


Figure 96. The FE-Mesh Parameters dialog window (Mesh Section Tab).

5.4. *Finite Element Mesh Refinement.*

The Finite Element Mesh Refinement is carried out in two steps:

1. One must first define the desired type of **FE Mesh Refinement** using the dialog window shown in Figure 97. Mesh refinement can be defined around **Points**, **Lines**, **Number of Points on the Line**, **Surfaces**, or **Solids**.
2. Next, users must assign the refinement to particular Points, Lines or Surfaces, so the program knows where the refinement should take place. After double clicking on a particular point, line, arc, circle or spline, the corresponding dialog window will appear (the **Edit Point** dialog window, Fig. 44; or the **Edit Curve** dialog window, Fig. 46), where users should select **FE-Mesh Refinement** in the **FE-Mesh Tab**. The code will then create a list of nodes (or lines or surfaces) for a particular refinement that can be further edited by a user. **FE Mesh Refinement** is graphically displayed using red dots in green circles for nodes, green nodes for lines, and a small square in the corner of a surface. By clicking on these colored items, the **FE Refinement** can be deleted or edited. Editing of the FE mesh refinement will affect all objects to which a particular refinement was assigned.

5.4.1. *Finite Element Mesh Refinement for MeshGen2D*

Figure 97 below shows the **New FE-Mesh Refinement** dialog windows that are used with the **MeshGen** module for four different types of refinements. **FE-Mesh Refinements** can be applied to a **Point**, a **Line**, and a **Surface**.

When the **FE-Mesh Refinement** is assigned to a **Point** (Figure 97 top left), users only need to define the finite element size that is to be used at a given point. This FE-size will be used around a given point, while sizes of neighboring FE will be gradually increased until the **Targeted FE Size** is reached further away in the computational domain. Notice that the dialog window also displays the **Global Targeted FE Size**. The same **FE-Mesh Refinement**, i.e., the same refined FE size, can be assigned to multiple **Points** in the transport domain.

There are two ways how the **FE-Mesh Refinement** can be assigned to a **Line** (Figure 97 top right and bottom left). Users can either specify the **FE-Size** (**Line – FE-Size;** Figure 97 top right) or the **Number of Points** (**Line – Number of Points**; Figure 97 bottom left) to be used on the entire line. Similarly as for points, the **FE-Size** (either given directly or calculated from the number of points) will be used on the **Line**, while sizes of FE away from the **Line** will gradually increased until the **Targeted FE Size** is reached further away in the computational domain. Again, the same **FE-Mesh Line Refinement**, i.e., the same refined FE size, can be assigned to multiple **Lines** in the computational domain.

The **FE-Mesh Refinement** can also be assigned to a selected **Surface** (Figure 97 bottom right). In this case, users need to define FE-Size for a selected **Surface**. Note that this option is useful only when multiple **Surfaces** are used in the computational domain. The refined FE-Size is then used on the entire surface, including boundaries with other **Surfaces**, and the **Targeted FE Size** is reached only further away in the other **Surfaces** of the computational domain.

The **Point** or **Surface** with an assigned **FE-Mesh Refinement** are indicated using the following marks: and , respectively. **FE-Mesh Refinement** is marked on curves using green points. visible in the edit mode site. Contrary to other green points on the curves, they can be selected.

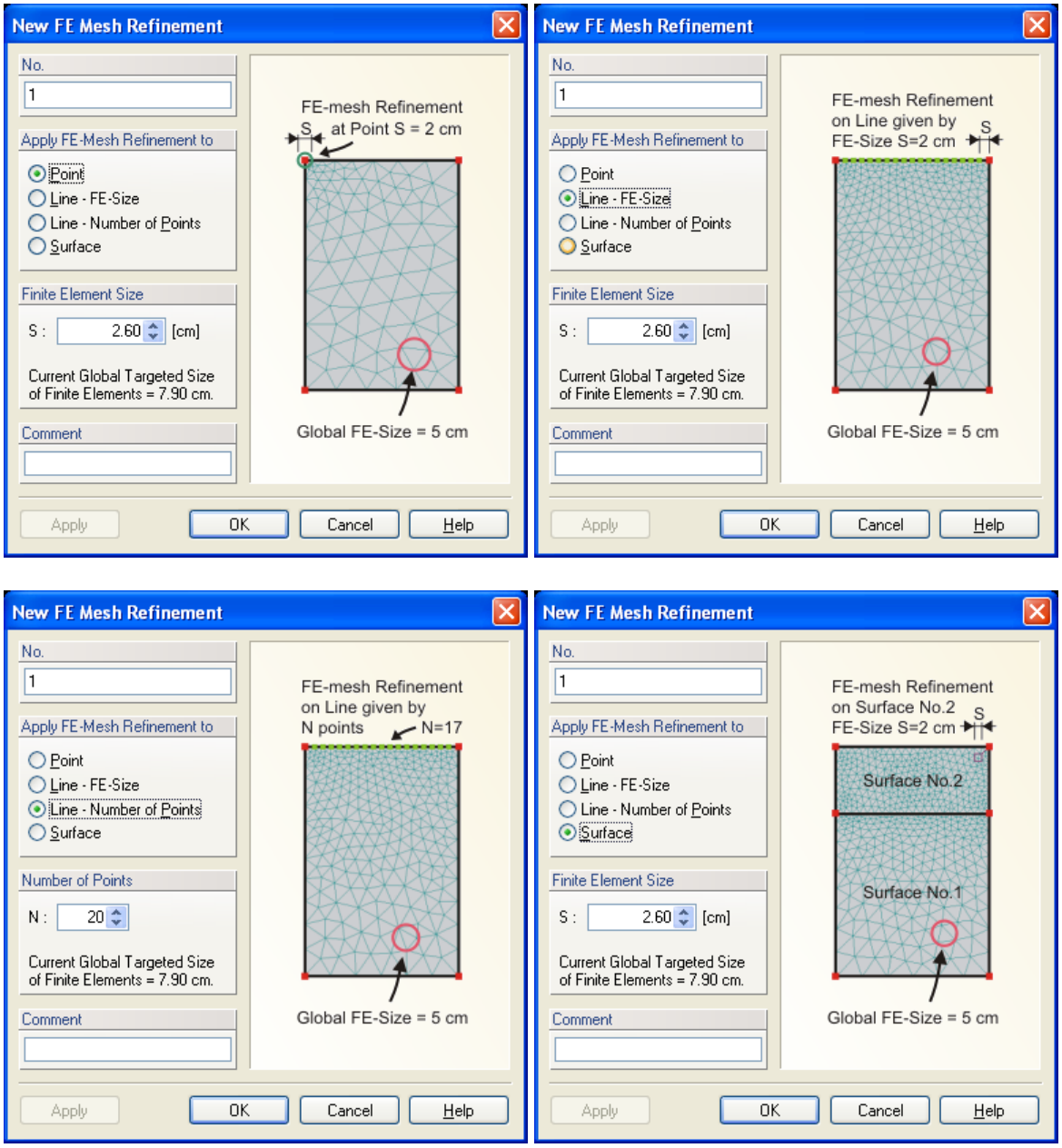


Figure 97. The FE-Mesh Refinement dialog window for the **MeshGen2D** module with four different types of refinements (applied to a Point, a Line with a given FE-size or the number of Points, and to a Surface).

As an example, Figure 98 shows the transport domain (700 * 650 cm) and the finite element mesh of a problem with a furrow and a drain. The mesh was generated with a **Targeted FE Size** of 50 cm and three **FE-Mesh Refinements** (Fig. 98, top). Refinement 1 (with a finite element

size of 10 cm) was assigned to nodes 1, 2, 4 and 5, refinement 2 (5 cm) to node 3, and refinement 3 (15 cm) to nodes 8 and 9. There were 15 nodes on the drain boundary (due to the command **Minimum Number of Points on Each Closed Boundary Curve**). The resulting finite element mesh is shown in Figure 98 (bottom).

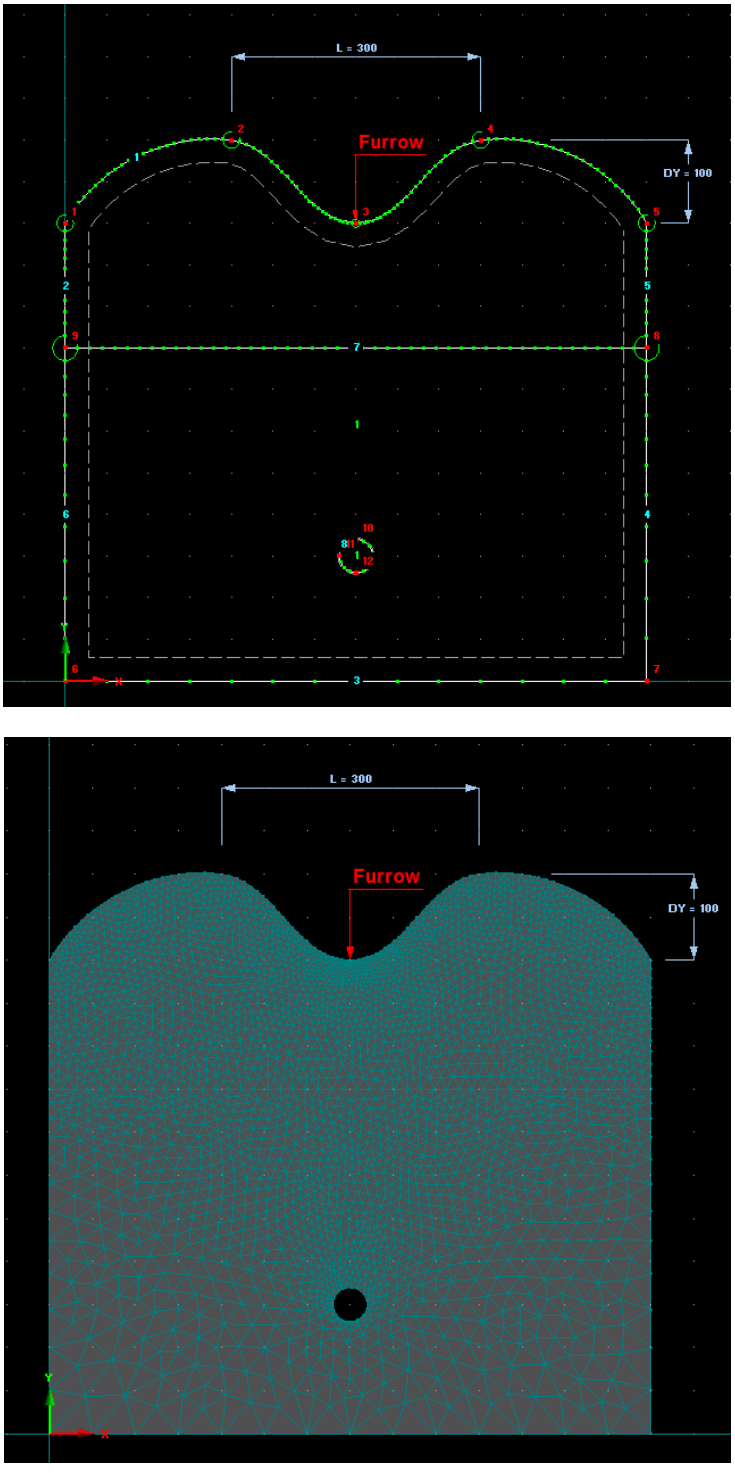


Figure 98. Example of FE-Mesh Refinements (top) and FE-Mesh (bottom).

5.4.2. *Finite Element Mesh Refinement for Genex/T3D*

While the **MeshGen2D** module discretizes the computational domain into unstructured FE-mesh using triangles (in 2D) and tetrahedrals (in 3D), the **Genex/T3D** module uses primarily quadrilateral (in 2D) and hexahedral (in 3D) finite elements. **Genex/T3D** uses triangles only in parts of the domain where needed, e.g., when it refines the grid. Although quadrilateral or hegahedral elements may be generated by **Genex/T3D**, the computational module subdivides these elements into triangles or tetrahedrals, respectively While the transition between domains with refined FE-mesh and domains with global mesh size in **MeshGen2D** is relatively smooth and gradual (see Figure 98), in **Genex/T3D** the extent of this transition zone is defined exactly by users (see Figures below). Similarly as **MeshGen2D**, the same **FE-Mesh Line Refinements** can be assigned to multiple **Points**, **Lines**, **Surfaces**, and **Solids** in the computational domain.

There are two ways how the **FE-Mesh Refinement** can be assigned to a **Point** (Figure 99). Users can use either **Circular** or **Rectangular** refinement. For a **Circular Refinement** around a point, a radial refinement area is defined around a node in all directions. Users need to specify the **Radius** of the refinement area, the **Inner Targeted FE-Size** (i.e., a FE-size immediately around a point), and the **Outer Targeted FE-Size** (i.e., a FE-size at the outer end of the radial refinement area) (Fig. 102). The **Outer Targeted FE-Size** should be equal or slightly smaller than the **Global Targeted FE-Size**. When generating the FE mesh, the mesh refinement is carried out gradually towards the center because the FE length at the periphery of the refinement area is usually identical with the global mesh width. For larger differences between the inner and outer FE length, it is recommended to set the radius not too small in order to avoid acute-angled triangular finite elements in the refinement area. For a **Rectangular Refinement**, a rectangular refinement area is defined around a node in all directions. Users need to specify the **Side Length** of the refinement area and the **Inner Targeted FE-Size** (i.e., a FE-size immediately around a point) (Fig. 102).

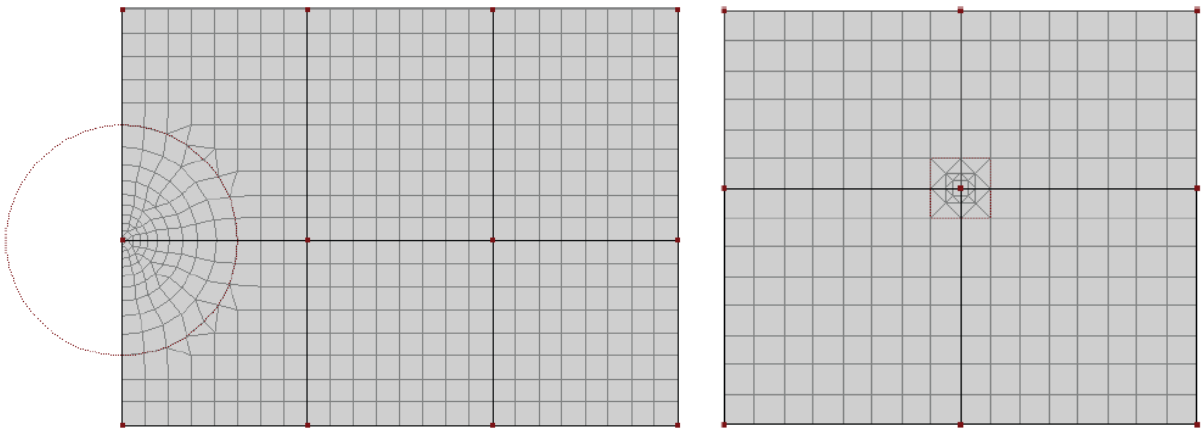


Figure 99. Circular (left) and rectangular (right) refinements around a node.

FE-Mesh Refinements assigned to a **Line** are handled in **Genex/T3D** similarly as in **MeshGen2D**. One can again define either the size (spacing; **Line through FE-Length**) or the number (a specific number of equidistant sub-divisions; **Line through Division**) of finite

elements along a line. In the former case one needs to define the **Target FE Length**, in the latter case the **Number of Division FE Nodes**. However, while in **MeshGen2D** there was a gradual increase in sizes of finite elements away from the **Line**, in **Genex/T3D** the refinement affects only one row of finite elements (Figure 100).

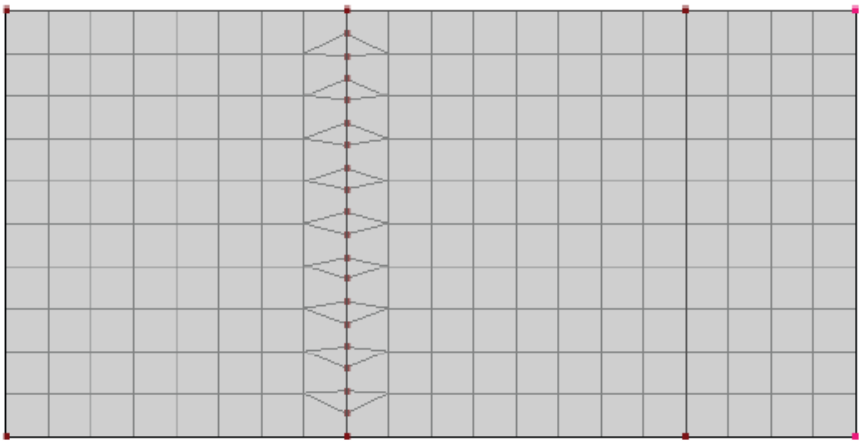


Figure 100. Refinement on a line (by defining either the size or the number of finite elements along a line).

It is also possible to define **Fe-Mesh Refinements** for **Surfaces** or **Solids** (Figure 101). In both cases, users need to specify the **Targeted FE-Size**, which will be set as target size of the finite elements for the entire surface or solid.

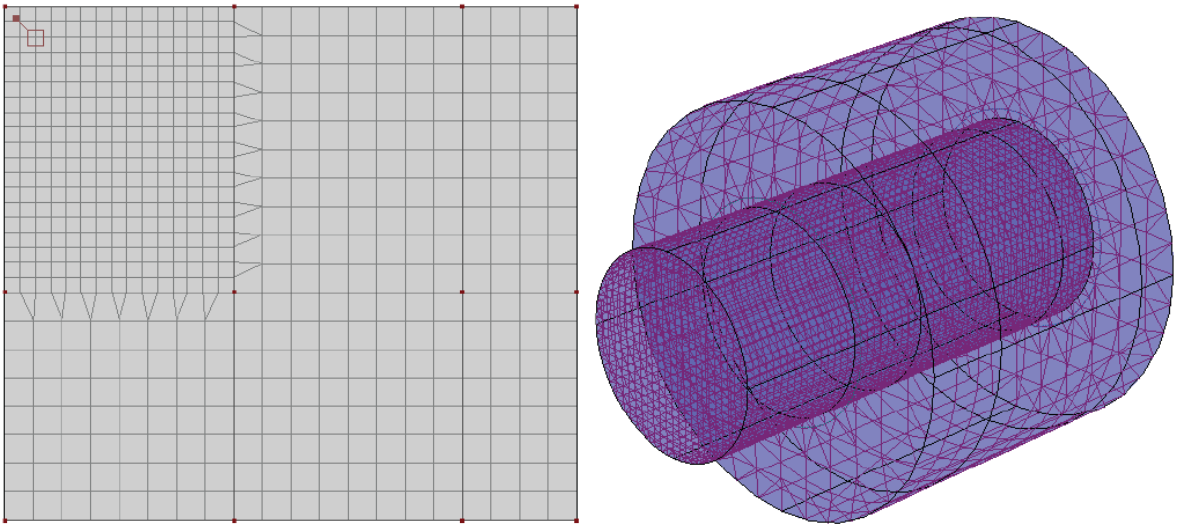
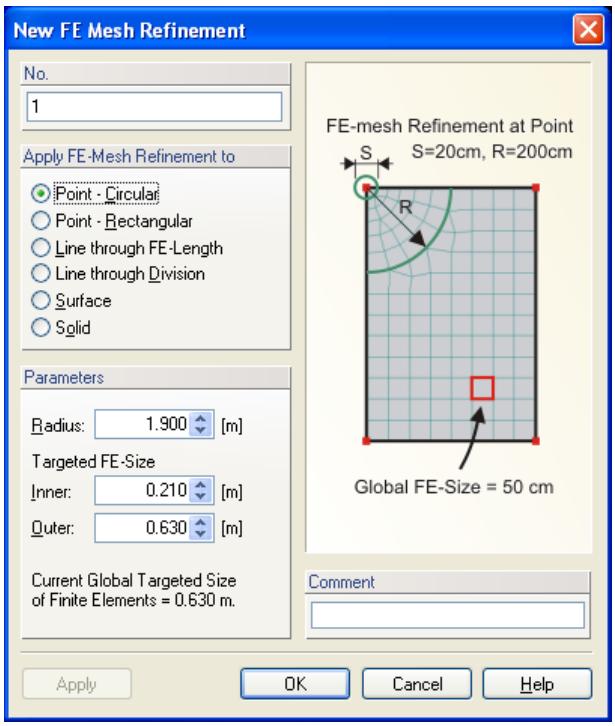
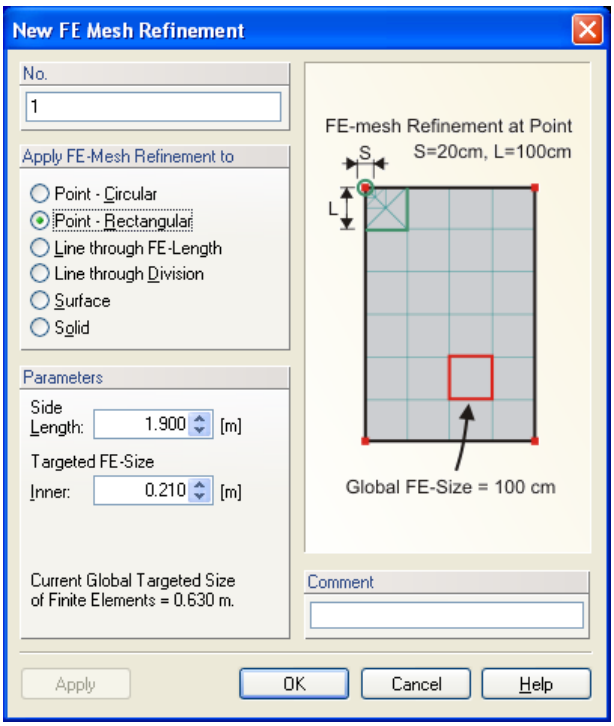
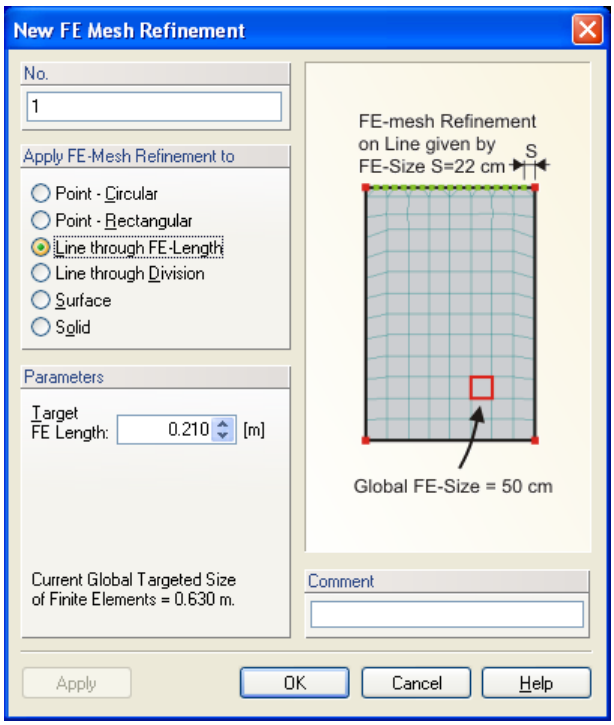
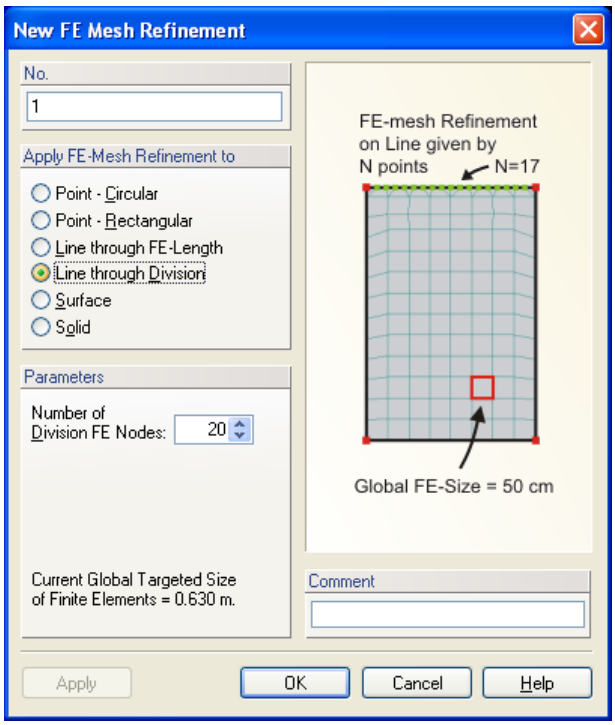


Figure 101. Refinements on a surface (left) or solid (right).


New FE Mesh Refinement
No.
1
Apply FE-Mesh Refinement to
Point - Circular
Point - Rectangular
Line through FE-Length
Line through Division
Surface
Solid
Parameters
Radius: 1.900 [m]
Targeted FE-Size
Inner: 0.210 [m]
Outer: 0.630 [m]
Current Global Targeted Size of Finite Elements = 0.630 m.
FE-mesh Refinement at Point
S=20cm, R=200cm
S
R
Global FE-Size = 50 cm
Comment
Apply
OK
Cancel
Help


New FE Mesh Refinement
No.
1
Apply FE-Mesh Refinement to
Point - Circular
Point - Rectangular
Line through FE-Length
Line through Division
Surface
Solid
Parameters
Side Length: 1.900 [m]
Targeted FE-Size
Inner: 0.210 [m]
Current Global Targeted Size of Finite Elements = 0.630 m.
FE-mesh Refinement at Point
S=20cm, L=100cm
S
L
Global FE-Size = 100 cm
Comment
Apply
OK
Cancel
Help


New FE Mesh Refinement
No.
1
Apply FE-Mesh Refinement to
Point - Circular
Point - Rectangular
Line through FE-Length
Line through Division
Surface
Solid
Parameters
Target FE Length: 0.210 [m]
Current Global Targeted Size of Finite Elements = 0.630 m.
FE-mesh Refinement on Line given by FE-Size S=22 cm
S
Global FE-Size = 50 cm
Comment
Apply
OK
Cancel
Help


New FE Mesh Refinement
No.
1
Apply FE-Mesh Refinement to
Point - Circular
Point - Rectangular
Line through FE-Length
Line through Division
Surface
Solid
Parameters
Number of Division FE Nodes: 20
Current Global Targeted Size of Finite Elements = 0.630 m.
FE-mesh Refinement on Line given by N points
N=17
Global FE-Size = 50 cm
Comment
Apply
OK
Cancel
Help

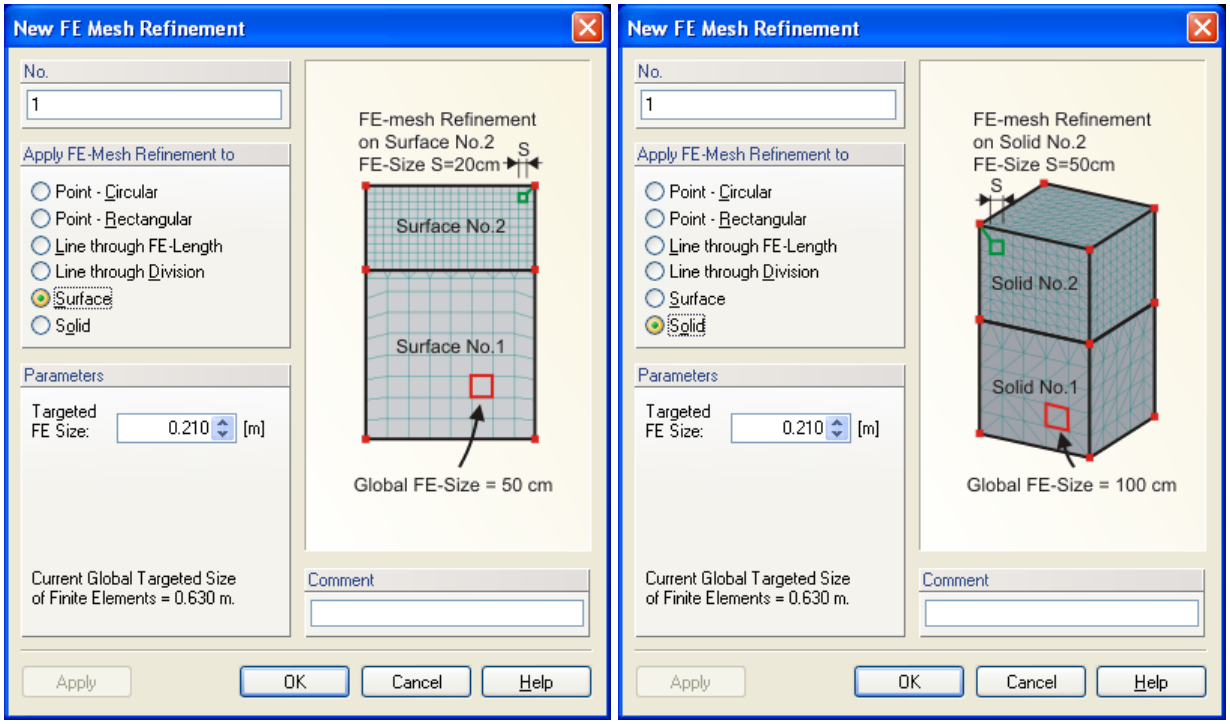


Figure 102. The **FE-Mesh Refinement** dialog window for the **Genex/T3D** module with six different types of refinements (applied to a **Circular** or a **Rectangular Point**, a **Line** with a given FE-size or a number of points, to a **Surface,** and to a **Solid**).

5.5. *Unstructured Finite Element Mesh Generator MeshGen2D*

The **MeshGen2D** module may be used to discretize a two-dimensional flow region (or a base plane of the three-dimensional domain) into an unstructured triangular mesh. The algorithm used for this purpose is general and can be applied to virtually any two-dimensional computational domain. The first step of the mesh generation process discretizes the boundary curves, while the second step generates the unstructured triangular mesh.

Generation of Boundary Points

The first step of the mesh generation process involves discretization of the boundary curves. During this step boundary nodes are generated on all boundaries and internal curves by dividing them in abscissas (i.e., short boundary edges). If no previous boundary nodes existed, the program automatically generates a default equidistant point distribution. Boundary nodes can be edited by users to optimize the lengths of the boundary edges using the **FE-Mesh Parameters** dialog window (Figs. 92 through 95). The local density of the mesh can thereby be determined in any part of the domain (also taking into account the use of internal curves). There are two ways to obtain appropriate distributions of the boundary nodes, i.e., by (1) specifying the *Targeted FE size* (Figs. 92, the Main Tab), and (2) refining the FE-Mesh (the **FE Mesh refinement** dialog window, Fig. 97).

1) A global **Targeted FE Size** (Fig. 92) is the main variable of the FE-Mesh process. Although a default Targeted FE-Size is specified by the program, this value should be adjusted by users in most applications. The default value is used to generate at least a reasonable initial mesh, even for inexperienced users.
2) The finite element mesh can be adjusted locally in the domain by using **FE-Mesh Stretching** (Fig. 93 and 103) or **FE-Mesh Refinement** (Figs. 44, 35, and 97). **FE-Mesh Refinement** can be implemented for various geometrical objects, including **Points**, **Lines** or **Surfaces** (Fig. 97). When several **FE-Mesh Refinements** overlap in one location (such as when the **FE-Mesh Refinement** is defined for both a point and a line), then the FE-Mesh Refinement specified for the lower level objects (i.e., a point rather than a line) is used.

The boundary nodal distribution determines in a very substantial manner the ultimate quality and size of the unstructured finite element mesh. Optimally distributing nodes along the boundaries of relatively complicated domains (e.g., a very irregular anisotropic domain) can be a very difficult problem, and may require some experience.

Table 18. Definition of terms related to the boundary discretization.

Boundary Nodes	Boundary nodes are points, marked by green squares, which discretize boundary curves. These nodes are generated along every boundary curve and are ordered in a counter-clockwise direction (on closed curves). Boundary nodes determine the local densities of the triangular mesh that is being generated for a given boundary nodal distribution, and are part of the triangular mesh.

Boundary Edges	Boundary edges are abscissas discretizing boundary curves. They connect generated boundary nodes, are oriented in a counter-clockwise direction, and are located on the edge of the mesh.
Fixed Points	Fixed points are points on boundary curves marked by red squares. These points may be used to adjust the local density of boundary nodes (using **FE Mesh refinement**). By default, fixed points are placed on all nodes of polylines and on all object boundary points describing the boundary, but they can be also inserted or deleted at any other point on boundary curves.

Generation of the Unstructured Triangular Mesh

The unstructured triangular mesh is generated by means of five operations:

(1) discretization of the flow domain into triangles with vertices at given boundary nodes (**Fundamental Triangulation**),
(2) inserting new points in all triangles which do not fulfill a certain smoothness criterion (**Mesh Refinement**),
(3) implementation of Delaunay's retriangulation for the purpose of eliminating all nodes surrounded by more than six triangles, as well as to avoid extreme angles (**Remeshing**),
(4) smoothing of the mesh by solving a set of coupled elliptic equations in a recursive manner (**Smoothing**), and
(5) correction of possible errors which may appear during smoothing of the finite element mesh (**Convexity Check**).

Operations 2 through 5 are repeated until a prescribed smoothness of the mesh has been achieved.

An unstructured triangular mesh for a given boundary nodal distribution can be generated in two different ways: a step-by-step approach (*Calculation->Advanced FE-Mesh Generation->Fundamental Triangulation* and subsequent commands, or by clicking on the **Fundamental Triangulation** command of the **FE-Mesh Advanced** part of the **FE-Mesh** version of the **Tool Sidebar**), or by using automatic mesh generation (*Calculation->Generate FE-Mesh* or the **Generate FE-Mesh** command on the **Edit FE-Mesh** part of the **FE-Mesh** version of the **Tool Sidebar**). The step-by-step approach should be used only for special cases, and then only by experienced users. Automatic generation (recommended) is a much faster and easier approach. The mesh generation parameters must be specified before the mesh generation process is started. By modifying the mesh generation parameters, users can influence the smoothness of the mesh (**Smoothing Factor**, Fig. 94), its anisotropy (Figs. 93 and 103), computational time, and the possible display of intermediate results, among other features. The most important mesh generation parameter is the "smoothing factor", which can significantly affect the final number of elements. The smoothing factor is defined as the ratio of the minimum and maximum dimensions of a triangle. When a very smooth finite element mesh is required, the smoothing factor should be decreased to about 1.1; when a coarser mesh is possible, the smoothing factor can be increased.

The code saves mesh data, by default, in a binary format (the file MESHTRIA.000). However, users have the option to also save mesh data into a file (MESHTRIA.TXT) in ASCII format (the Program Option dialog window, Fig. 150), and then use possibly the data later for other calculations.

When users do not have authorization to use the MeshGen2D module, they can employ the internal mesh generator for relatively simple rectangular or hexahedral transport domains.

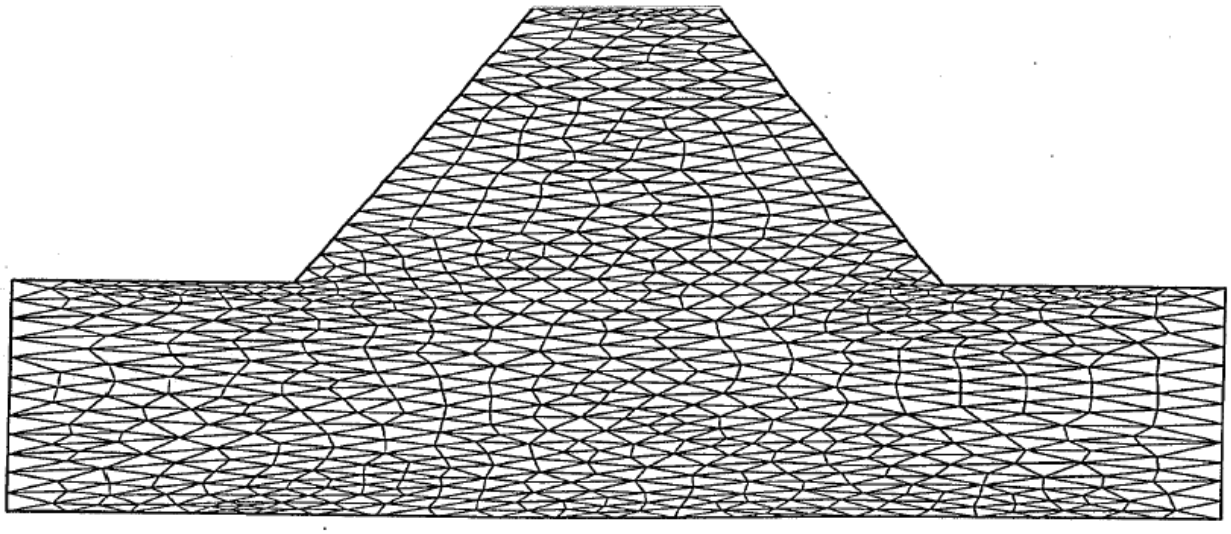


Figure 103. Example of mesh stretching using a stretching factor of 3 in the *x*-direction.

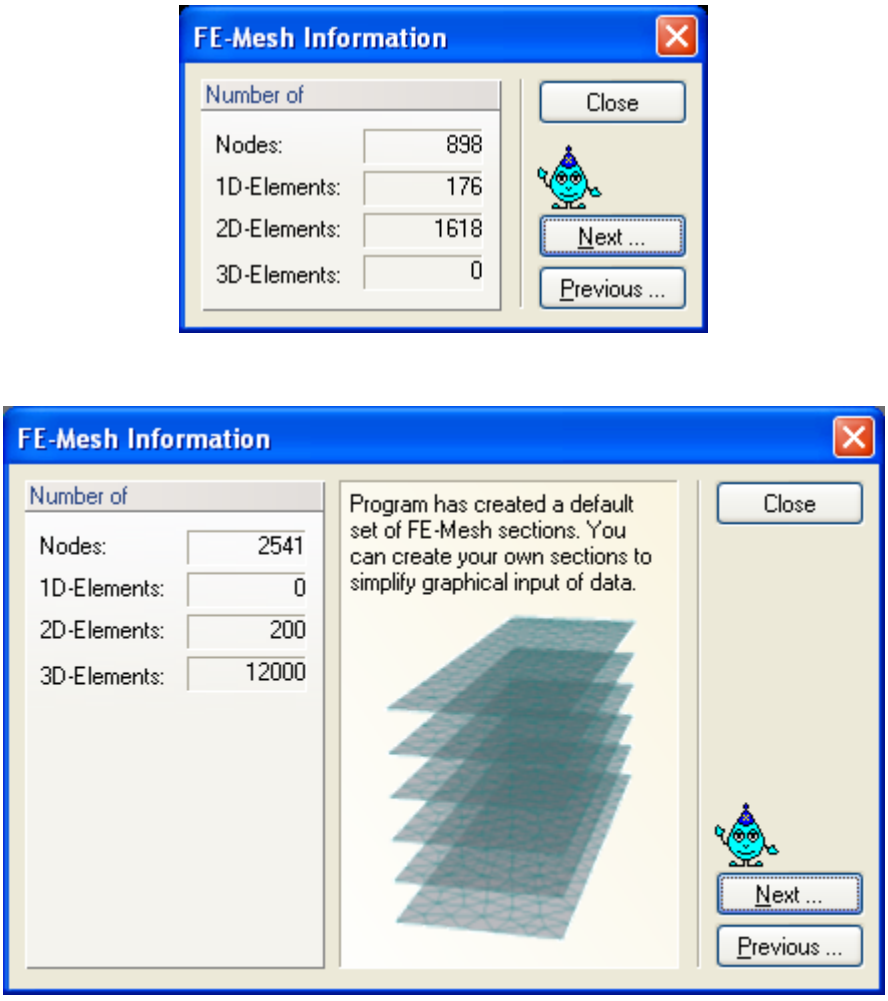


Figure 104. The FE-Mesh Information dialog window for a two-dimensional problem (top) and a three-dimensional problem (bottom).

Figure 104 shows dialog windows that provide information about the finite element mesh for two- and three-dimensional applications. For two-dimensional grids the window shows the number of finite element *Nodes*, the number of boundary *1D-Elements* (boundary edges between boundary nodes), and the number of *2D-Elements* (triangles). For three-dimensional grids the window shows again the number of finite element *Nodes* (in the entire 3D domain), the number of boundary *1D-Elements* (boundary edges between boundary nodes on the bottom plane, i.e., the 2D base surface of the transport domain), the number of *2D-Elements* (the number of triangles on the bottom plane of the domain), and the number of 3*D-Elements* (tetrahedrals) in the entire transport domain.

5.7. *Finite Element Mesh Sections*

FE-Mesh Sections are parts of the FE-Mesh used to specify input variables and to display results of calculations. By default, two-dimensional problems have only one section consisting of the entire transport domain. For three-dimensional problems one section by default is formed by the *Whole FE-Mesh* (Section D0_000 in Fig. 105), whereas each horizontal (vertical for some applications) layer forms one additional section (Sections ML_001 through ML_010 – *Mesh Layer* in Fig. 105), while the last section is made up by the vertical surface (Section ML_000 *Shell* Fig. 105). For example, the bottom Mesh Layer can be displayed when the bottom boundary conditions are specified, while the top Mesh Layer (Section) can be displayed when the surface boundary conditions are provided. One can similarly display results at different depths using different horizontal sections (Mesh Layers). The **Mesh Sections** are generated automatically when the FE-Mesh is generated or anytime using the menu command *Edit->Sections->Generate FE-Mesh Sections*. Automatically generated FE-Mesh Sections in different HYDRUS versions are listed in Table 19. Mesh Sections can also be generated for each Geo-Section (see Section 8.1.8).

Additional sections can be created using commands from the **FE-Mesh Sections** part of the **FE-Mesh** version of the **Edit Bar**. One can display any existing section (or set of sections) and modify them using the *Cut with Rectangle* command, and then create a new section using the *New Section from View* command. This new section will then appear in the list of sections in the **Section** Tab of the **Navigator Bar** and can be recalled at any time. Existing sections can be manipulated (*Display*, *Hide*, *Select*, *Unselect*, *Rename*, *Delete*, *Move Up*, and *Move Down*) using the *Edit Section* command from the **Edit Bar**, or using *Edit->Sections->Edit Sections*.

Table 19. Finite element mesh sections generated in different HYDRUS versions.

HYDRUS Version	**Generated FE-Mesh Sections**
2D-Lite	Nothing
2D-Standard	For each Surface (of more than one) and each Geo-Section (see Section 8.1.8) defined by user.
3D-Lite	For each layer of the FE-Mesh
3D-Standard	For each FE layer, each geometrical layer, and for each Column
3D-Professional	For each Geo-Section as defined in Section 8.1.8.

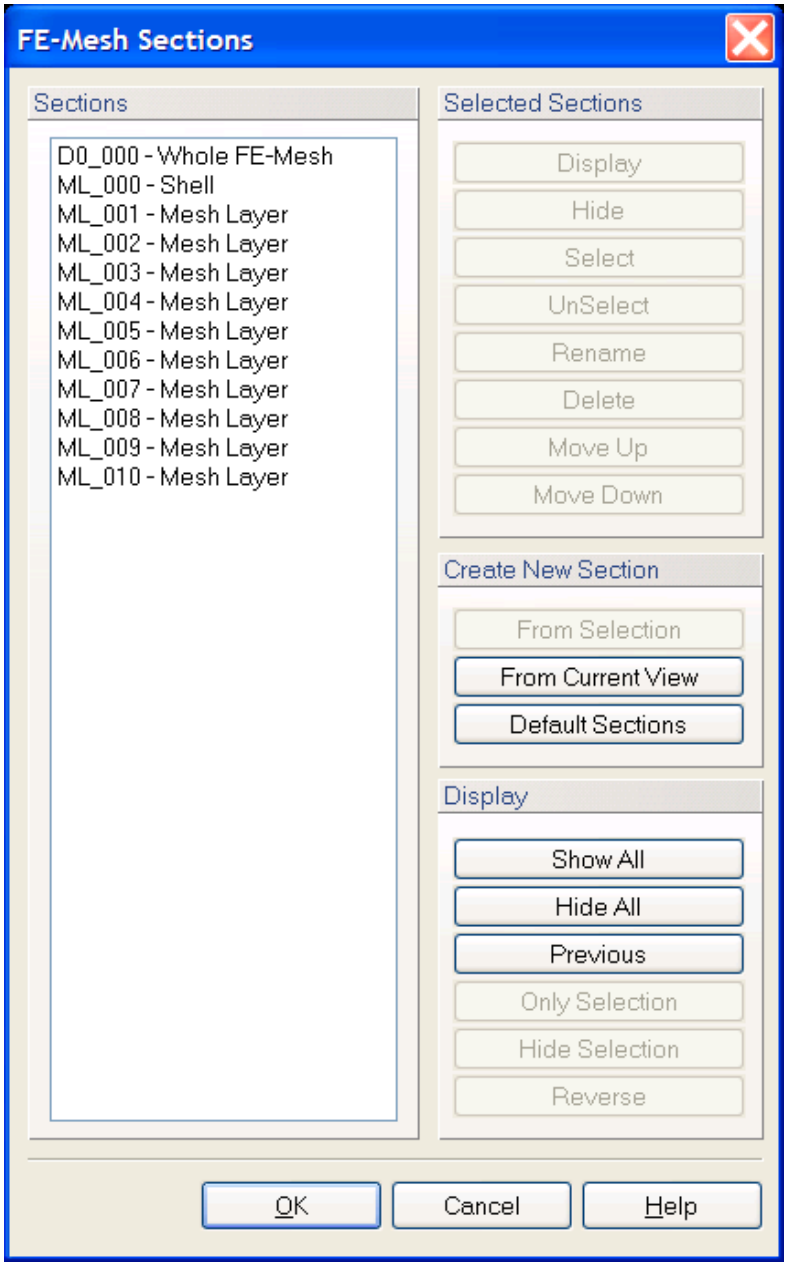


Figure 105. The FE-Mesh Sections dialog window.

6. Domain Properties, Initial and Boundary Conditions

Initial and boundary conditions for both water flow and solute (heat) transport, and the spatial distribution of other parameters characterizing the flow domain (e.g., the spatial distribution of soil materials, hydraulic scaling factors, root-water uptake parameters, and possible hydraulic anisotropy) and/or observation nodes are specified in a graphical environment with the help of a mouse. The program automatically controls the logical correspondence between the water flow and solute transport boundary conditions.

Various spatially variable properties (e.g., material distribution, initial and boundary conditions) can be specified in Version 2.0 of HYDRUS (Standard and Professional, not Lite) either

a) directly on the finite element mesh (as done in Version 1.0), or
b) on geometrical objects (e.g., boundary curves, rectangles, circles, surfaces, volumes).

The main advantage of the latter approach is that when the FEM is changed, these properties are not automatically lost, but can be recalculated to the new FEM from their definition on Geometrical Objects. Which option is used depends on the menu command *Edit->Properties and Conditions on FE-Mesh*. A similar button switch is also available at the end of the tool bar ( ), next to the Results button, and at the Edit Bar. The latter approach (i.e., on Geometrical Objects) is described in detail below in Section 6.5.

6.1. *Default Domain Properties*

For rectangular two-dimensional domains and for layered three-dimensional domains, immediately after the finite element mesh is generated, one can specify the initial **Default Domain Properties** in the dialog window shown in Figure 106. Values listed in this window are initially assigned to each horizontal layer of the transport domain, but can later be modified graphically. The following variables are involved:

Code Code of the boundary condition (0 for no flow, -1 for constant flux, +1 for constant head, -2 for unsaturated seepage face, +2 for saturated seepage face, -3 (-7, -8, -9) for variable flux, +3 (+7, +8, +9) for variable head, -4 for atmospheric, - 5 for tile drain, -6 for free drainage)

h Initial value of the pressure head [L]. The initial pressure head changes linearly between the first and last layer if one clicks on the command at the bottom of the dialog (*Linear interpolation of the pressure heads between the first and last layer*).

Q Recharge flux, [L^2T^{-1}] and [L^3T^{-1}] for 2D and 3D applications, respectively

Mater Material number

Roots Root distribution

Axz Scaling factor for the pressure head

Bxz Scaling factor for the hydraulic conductivity

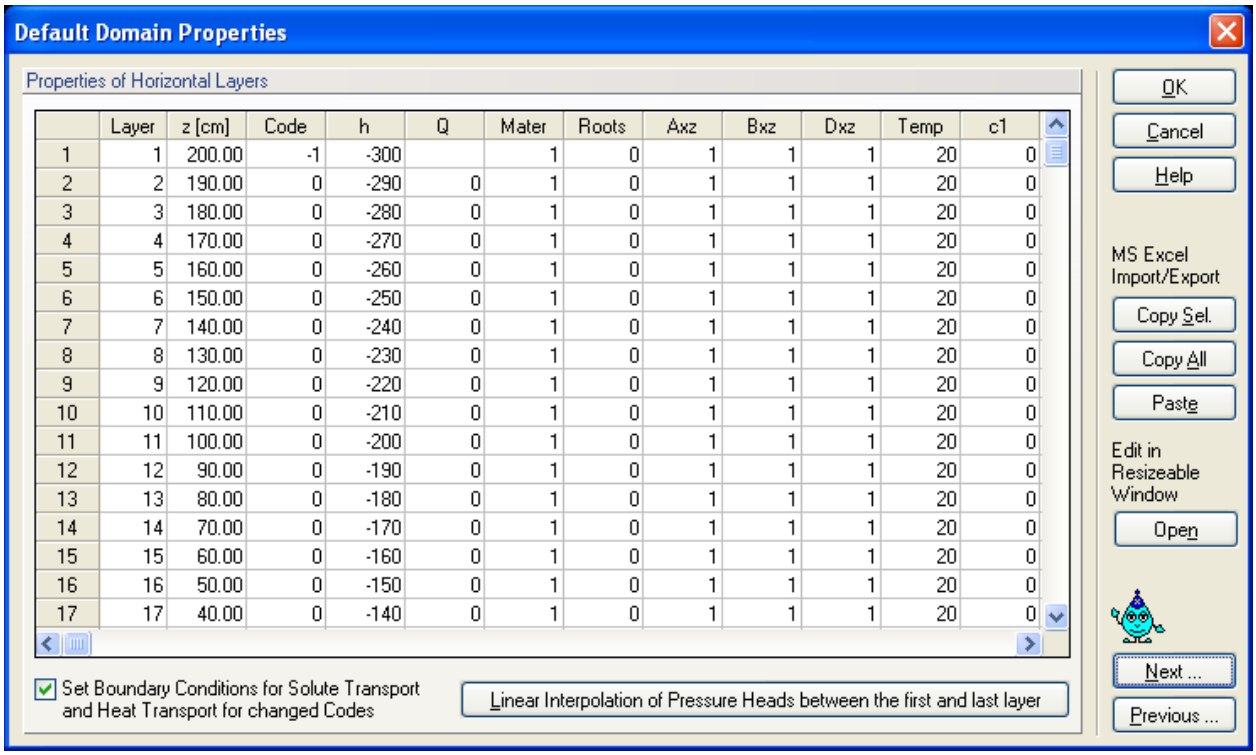
Dxz Scaling factor for the water content

Temp Initial temperature [K]

Conc Initial concentration (of the equilibrium phase) [ML^{-3}]

Sorb Initial concentration of the nonequilibrium phase (kinetically sorbed [MM^{-1}] or of the immobile region [ML^{-3}])

Values from each line are assigned to the entire layer within the FE-Mesh with the exception of Code (the boundary condition code), which is assigned only to boundary nodes. When multiple values are encountered within the single layer when initiating the table, the cell is left empty instead of displaying any particular value. Unless changed, this variable will not be assigned in a particular layer (after closing the dialog with OK) and original values will remain unchanged. The three commands (*Copy Sel.*, *Copy All*, and *Paste*, **MS Excel Import/Export**) facilitate the transfer of data from this HYDRUS dialog window to the Excel (or other) spreadsheet. The command "**Set Boundary Conditions for Solute Transport and Heat Transport for changed Codes**:" leads to assigning Cauchy boundary conditions for solute and heat transport to nodes where the Code was changed.



	Layer	z [cm]	Code	h	Q	Mater	Roots	Axz	Bxz	Dxz	Temp	c1
1	1	200.00	-1	-300		1	0	1	1	1	20	0
2	2	190.00	0	-290	0	1	0	1	1	1	20	0
3	3	180.00	0	-280	0	1	0	1	1	1	20	0
4	4	170.00	0	-270	0	1	0	1	1	1	20	0
5	5	160.00	0	-260	0	1	0	1	1	1	20	0
6	6	150.00	0	-250	0	1	0	1	1	1	20	0
7	7	140.00	0	-240	0	1	0	1	1	1	20	0
8	8	130.00	0	-230	0	1	0	1	1	1	20	0
9	9	120.00	0	-220	0	1	0	1	1	1	20	0
10	10	110.00	0	-210	0	1	0	1	1	1	20	0
11	11	100.00	0	-200	0	1	0	1	1	1	20	0
12	12	90.00	0	-190	0	1	0	1	1	1	20	0
13	13	80.00	0	-180	0	1	0	1	1	1	20	0
14	14	70.00	0	-170	0	1	0	1	1	1	20	0
15	15	60.00	0	-160	0	1	0	1	1	1	20	0
16	16	50.00	0	-150	0	1	0	1	1	1	20	0
17	17	40.00	0	-140	0	1	0	1	1	1	20	0

Figure 106. The Default Domain Properties dialog window.

6.2. *Initial Conditions*

After selecting nodes (graphically with the mouse) for which the initial condition is to be specified, and clicking on the command **Set Values** at the **Edit Bar** (on the right side of the view window), the **Water Flow Initial Condition** dialog window (Fig. 107) appears. Using this command one can specify the initial conditions for water flow by defining the initial spatial distribution of the pressure head or water content over the flow domain. The decision whether to use the pressure head or the water content initial distribution is made in the main module of the **Iteration Criteria** dialog window (Fig. 17). One can specify a) the same value to all selected nodes (*Same value for all nodes*), b) a distribution versus depth that is in equilibrium with the

pressure head of the lowest point in the selected region (*Equilibrium from the lowest located nodal point*), and c) a *Linear distribution with depth*. When options a) or b) are selected, only one value of the pressure head needs to be specified. For option c) one needs to provide values of the pressure head (or water content) for the top and bottom of the selected domain.

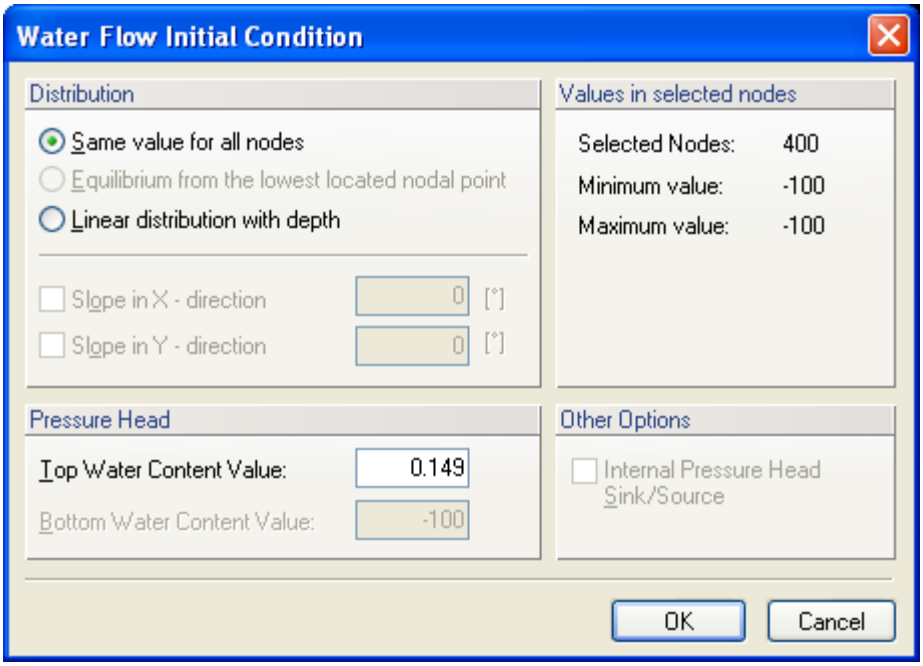


Figure 107. The Water Flow Initial Condition dialog window.

To simplify definition of the initial condition for problems that involve slopes, an option is provided to have pressure heads decrease in the *x*- and *y*- (the latter only for three dimensional problems) directions (*Slope in X- direction* and *Slope in Y- direction*).

The right top part of the dialog window (*Values in selected nodes*) in Figure 107 provides information about the selected nodes, i.e., the number of selected nodes and the minimum and maximum values of the pressure head or water content.

If a certain node is selected that is not located on the boundary, this node can be declared an *Internal Pressure Head Sink/Source*. The pressure head at that node will then be kept constant during the simulation.

Similar, but simpler, dialog windows are used to specify initial values of the temperature and the liquid and adsorbed concentrations (e.g., **Temperature Distribution** dialog window, Fig. 108). The dialog window will then again provide information about the selected nodes (*Values in selected nodes*), i.e., the number of selected nodes and their minimum and maximum temperatures (concentrations). One can specify either constant value for all selected nodes, or have the values change linearly with depth. When the box *Use top value for the entire selected region* is checked, the value in the *Top* box is assigned to all selected nodes.

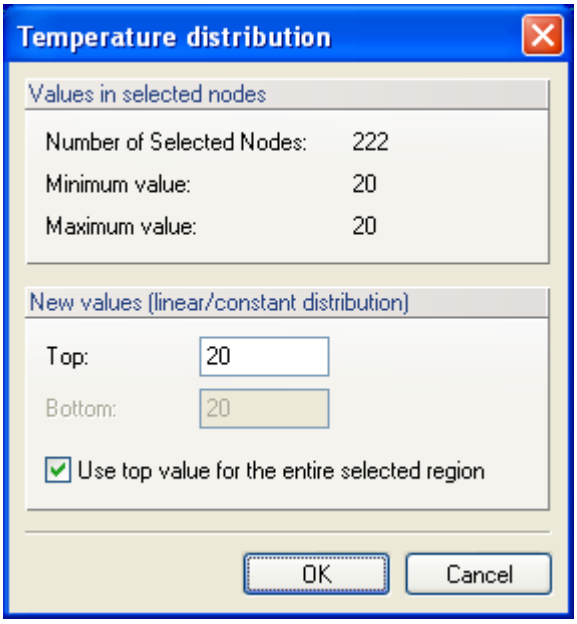


Figure 108. The Temperature distribution dialog window.

The initial condition can be imported from the results of previous calculations using the Import command (*Edit->Initial Condition->Import*, or *Insert->Initial Condition->Import*). After clicking on any of these two commands, an **Open** dialog window appears with **Files of type** preselected for HYDRUS applications (i.e.,*.h3d2). One then needs to browse for the HYDRUS project from which the initial condition is to be imported. After selecting a particular project, the **Import Initial Conditions** dialog window appears (Fig. 109). This window provides information from which project the initial conditions will be imported (*Import data from Hydrus project*) and offers quantities that can be imported as initial conditions (*Select quantities to import*). Users must then also decide in the *Select Time Layer* part of the dialog if values for *The Last (Final) Time Layer* or for any intermediate time layer (using *Time Layer No.:* from the lower list box) are to be imported. *Time Layers* correspond with **Print Times** (Fig. 16) for which the output in the existing project was calculated.

Warning: Import of results of previous calculations as initial conditions for the new simulation can be done only from a project that has an identical FE-Mesh discretization as the actual project!

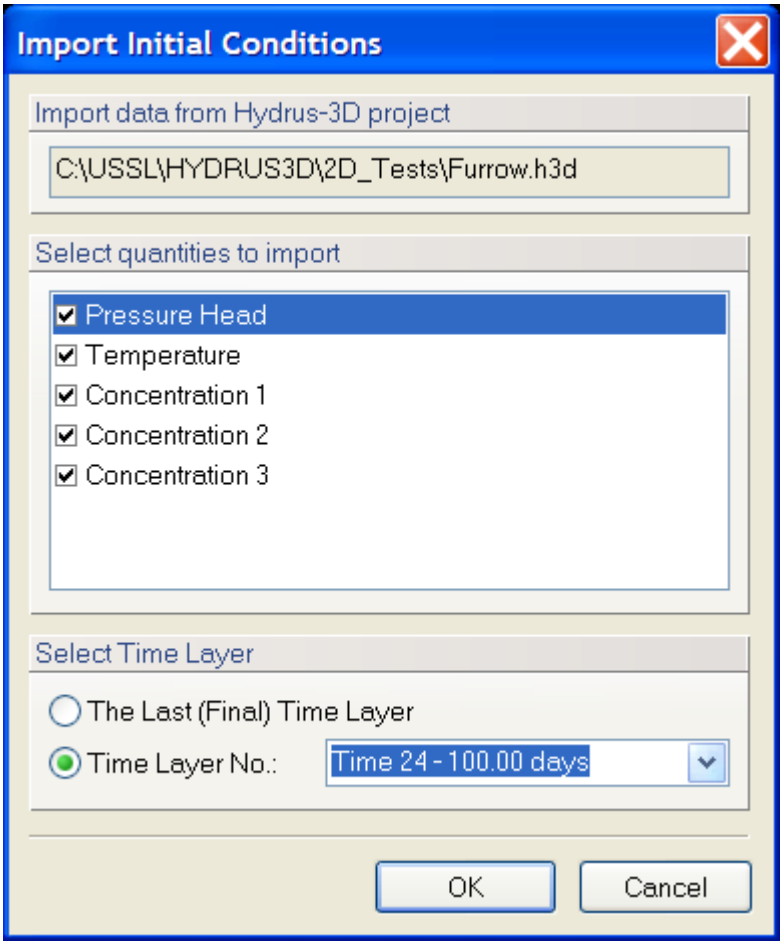


Figure 109. The Import Initial Condition dialog window.

6.3. *Boundary Conditions*

Specification of the boundary conditions is relatively straightforward. Users must first select from the **Navigator Bar** particular **Boundary Conditions** (i.e., water flow, solute transport, or heat transport) and then click on the **Edit Bar** on the particular boundary condition (e.g., constant head). They subsequently need to move the mouse to the selected position and click the left mouse button. Implementation of the boundary condition terminates with a repeated click of the left mouse button. The boundary nodes will acquire the same color as the corresponding type of the boundary condition. See the rules for specifying boundary conditions as described in Chapter 8 of the Technical Manual [*Šimůnek et al.*, 2010]. Alternatively, users can first select boundary nodes and then assign desired boundary conditions by clicking at a particular boundary condition at the **Edit Bar**. Note that the Free Drainage and Deep Drainage boundary conditions cannot be specified simultaneously in one project. Similarly, when the Gradient Boundary Conditions is specified (see description below), the Time-Variable Flux 4 Boundary Condition is disabled.

In addition to system-dependent boundary conditions available in version 2.x of HYDRUS-2D, several new options are available in HYDRUS. These new options are specified in the **Boundary Condition Options** dialog window (Fig. 110) that is called using the menu command *Edit->Boundary Conditions->Boundary Conditions Options* or from the **Edit Bar** for **Water Flow Boundary Conditions version** using the **BDRC Options** command. This dialog window has three tabs: a) **Time-Variable Head/Flux 1 BCs**, b) **Special Boundary Conditions**, and c) **Triggered Irrigation**.

6.3.1. *Time-Variable Head/Flux 1 BCs*

The options that are available on the first tab (**Time-Variable Head/Flux 1 BCs**, Fig. 110) apply to the first Time-Variable Head/Flux boundary condition. The following new options are available here:

a) While in version 2.0 of HYDRUS-2D, all boundary conditions (i.e., fluxes or pressure heads) changed in abrupt steps, the new version allows boundary pressure heads to change smoothly with time. Abrupt changes in the pressure heads lead to sudden changes in fluxes, while smoothly changing pressure heads provide smoothly changing fluxes. An example of such a boundary condition is the water level in a stream or furrow.

b) While version 2.0 of HYDRUS-2D only allowed either time-variable pressure heads or time-variable fluxes on a particular part of the boundary, the new version allows boundary conditions to change from variable pressure heads to a zero flux and vice-versa. This boundary condition can be used for example for a disc permeameter where the specified head changes to a zero flux during time periods when the permeameter is re-supplied with water. The zero flux is initiated by specifying a value larger than 999999.

c) When a time-variable pressure head boundary condition is specified along a boundary, then the specified value is assigned to the lowest nodal point of a particular boundary, while pressure heads at other nodes are adjusted based on the *z*-coordinate. When this option is selected, then nodes with calculated negative pressure heads are not associated with a Dirichlet boundary condition, but rather with a zero flux. A fluctuating water level in a stream or furrow is an example of this type of boundary condition. While positive pressure head values are below the water table, negative values occur above the water table.

d) This is similar to c) except that an atmospheric boundary condition is assigned to nodes with negative calculated pressure heads.

e) This is similar to c) except that a seepage face boundary condition is assigned to nodes with negative calculated pressure heads.

f) When this type of system-dependent boundary condition is selected, then HYDRUS treats the time-variable flux boundary conditions similarly as atmospheric fluxes. This means that pressure heads have two limiting values, with the maximum pressure head equal to hCritS and the minimum pressure head equal to hCritA.

g) While in version 2.x of the code, the flux across the nonactive part of the seepage face was always equal to zero, the new version can apply atmospheric boundary conditions on a nonactive seepage face.

h) When heat transport is simulated simultaneously with water flow and atmospheric boundary conditions, then snow accumulation on top of the soil surface can be simulated. The code then assumes that when the air temperature is below -2 C all precipitation is in the form of snow. When the air temperature is above +2 C all precipitation is in the form of liquid, while a linear transition is used between the two limiting temperatures (-2,2). The code further assumes that when the air temperature is above zero, the existing snow layer (if it exists) melts proportionally to the air temperature.

Boundary condition options a) through g) can be used only with the first time-variable head condition.

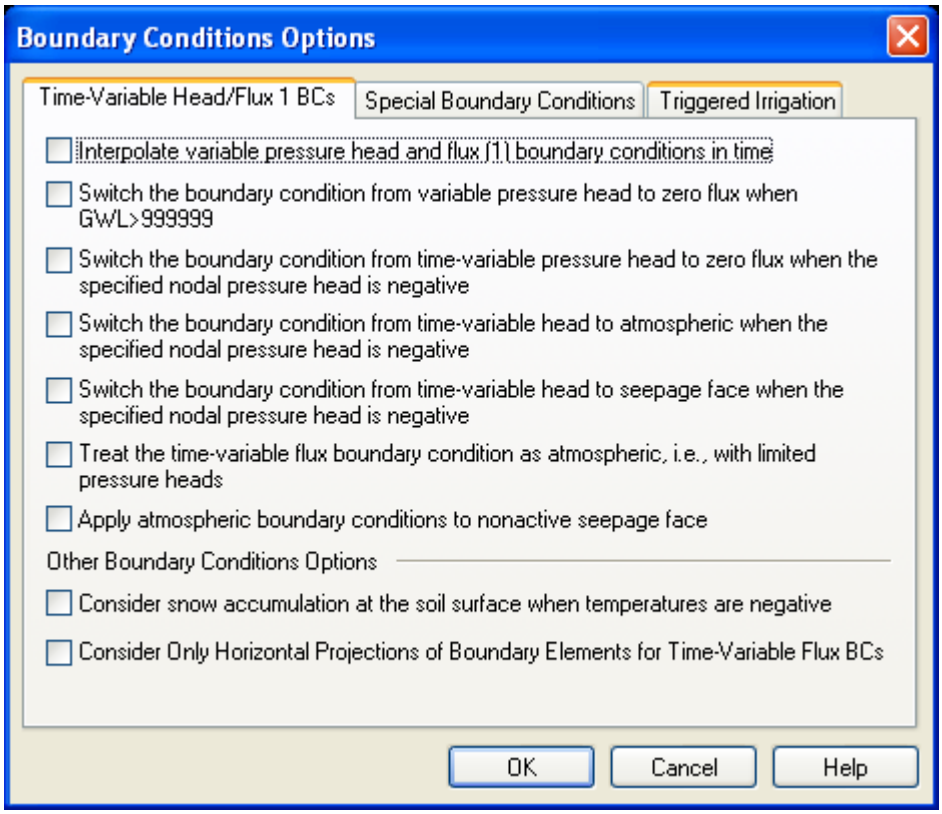

Boundary Conditions Options
Time-Variable Head/Flux 1 BCs
Special Boundary Conditions
Triggered Irrigation
Interpolate variable pressure head and flux (1) boundary conditions in time
Switch the boundary condition from variable pressure head to zero flux when GWL>999999
Switch the boundary condition from time-variable pressure head to zero flux when the specified nodal pressure head is negative
Switch the boundary condition from time-variable head to atmospheric when the specified nodal pressure head is negative
Switch the boundary condition from time-variable head to seepage face when the specified nodal pressure head is negative
Treat the time-variable flux boundary condition as atmospheric, i.e., with limited pressure heads
Apply atmospheric boundary conditions to nonactive seepage face
Other Boundary Conditions Options
Consider snow accumulation at the soil surface when temperatures are negative
Consider Only Horizontal Projections of Boundary Elements for Time-Variable Flux BCs
OK
Cancel
Help

Figure 110. The Time-Variable Head/Flux 1 BCs tab of the Boundary Condition Options dialog window.

6.3.2. *Special Boundary Conditions*

The following **Special Boundary Conditions** (Fig. 111) can be selected from the second tab of the **Boundary Condition Options** dialog window:

1. Gradient Boundary Conditions
2. Subsurface Drip Characteristic Function
3. Surface Drip Irrigation with a Dynamic Evaluation of the Wetted Area
4. Seepage Face with a Specified Pressure Head

Gradient Type Boundary Condition

Version 1 of HYDRUS implements the **Gradient Type Boundary Condition** only as the **Free Drainage** boundary condition, or the unit gradient boundary condition. However, in many situations one needs a non-unit gradient BC. For example, it is difficult to select appropriate boundary conditions for vertical boundaries for flow in a hill slope where the side-gradient is more or less parallel with the direction of the slope. In version 2 of HYDRUS, users can specify a gradient other than one (unit gradient). This option, i.e., non-unit gradient boundary condition, needs to be selected from the **Special Boundary Conditions** tab of the **Boundary Conditions Options** dialog window. Gradients are positive for flow against a particular axis, i.e., from right to left (in the *x*-direction) and from back to front (in the *y*-direction), and should be used only (or mainly) on sides of the transport domain. In 3D, the gradient BC can be specified only in one direction (i.e., either in *x*- or *y*-direction).

Subsurface Drip Characteristic Function

Infiltration rate of water from a subsurface cavity (dripper) is affected by many factors, including the pressure in the cavity, its size and geometry, and the hydraulic properties of the surrounding soil [*Lazarovitch et al.*, 2005]. When a predetermined discharge of a subsurface source (e.g., a subsurface emitter) is larger than the soil infiltration capacity, the pressure head in the source outlet increases and becomes positive. The built up pressure may significantly reduce the source discharge rate. A special system-dependent boundary condition for flow from subsurface sources that uses the drip characteristic function was implemented in HYDRUS (see the Technical manual). This function has two variables, i.e., the nominal discharge (**Optimal Flux** in Fig. 111) of the source for the reference inlet pressure h_{in} (usually being 10 m) and the back pressure equal to zero, and an empirical constant (**Exponent** in Fig. 111) that reflects the flow characteristics of the emitter. Normally, c = 0.5 corresponds to a turbulent flow emitter and c = 1 to a laminar one.

Implementation: User needs to specify the "**Time-Variable Flux 1**" boundary condition along the dripper boundary and h_{in} in the "**Var.H-1**" column of the "**Time Variable Boundary Conditions**" dialog window. A positive pressure indicates an irrigation period and a negative pressure indicates a non-irrigation period.

Surface Drip Irrigation – Dynamic Evaluation of the Wetted Area

The radius of the wetted area for drip irrigation for transient conditions can be calculated in Hydrus as follows. The irrigation flux Q is applied to the single boundary node that represents the dripper with the Neumann (flux) boundary condition. If the pressure head required to accommodate the specified flux Q is larger than zero, the boundary condition in this particular node is changed into the Dirichlet (head) boundary condition with zero pressure head value and the actual infiltration flux Q_a through this node is calculated. The excess flux (Q - Q_a) is then

applied to the neighboring node, again with the specified Neumann boundary condition. This procedure is iteratively repeated until the entire irrigation flux *Q* is accounted for and the radius of the wetted area is obtained. Since the infiltration flux into the dry soil is larger for early times, the wetted area continuously increases as irrigation proceeds.

Implementation: User needs to specify the "**Time-Variable Flux 1**" boundary condition at the surface boundary. The length of this boundary needs to be sufficient to accommodate the entire wetting zone. The drip discharge flux, *Q*, needs to be entered in the "**Var.Fl-1**" column of the "**Time Variable Boundary Conditions**" dialog window. User also needs to specify from which node of the **Time-Variable Flux 1** boundary irrigation starts. Irrigation can start in the left node of the boundary and then the wetting zone will be spreading to the right (**From left to right**), it can also starts in the right node of the boundary and then the wetting zone will be spreading to the left (**From right to left**), or it can start in the arbitrary middle node of the boundary (**Center Node**) and spread in both direction (**From the center**).

Seepage Face with a Specified Pressure Head

This type of boundary condition is often applied to laboratory soil columns when the bottom of the soil column is exposed to the atmosphere (gravity drainage of a finite soil column). The condition assumes that the boundary flux will remain zero as long as the pressure head is negative. However, when the lower end of the soil profile becomes saturated, a zero pressure head is imposed at the lower boundary and the outflow calculated accordingly. This type of boundary condition is often used for lysimeters.

User can specify a pressure head value other than zero (**Pressure Head**) for triggering flux across the seepage face (in several experimental settings, a negative pressure can be applied at the bottom of laboratory columns or lysimeters).

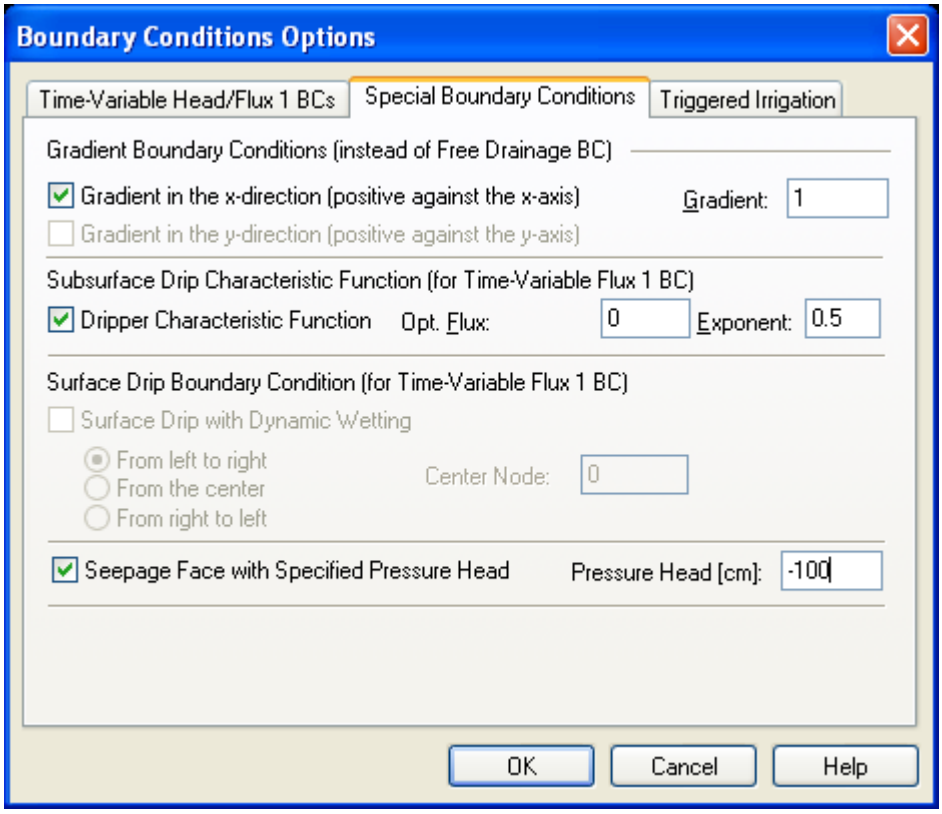

Boundary Conditions Options
Time-Variable Head/Flux 1 BCs
Special Boundary Conditions
Triggered Irrigation
Gradient Boundary Conditions (instead of Free Drainage BC)
Gradient in the x-direction (positive against the x-axis)
Gradient: 1
Gradient in the y-direction (positive against the y-axis)
Subsurface Drip Characteristic Function (for Time-Variable Flux 1 BC)
Dripper Characteristic Function
Opt. Flux: 0
Exponent: 0.5
Surface Drip Boundary Condition (for Time-Variable Flux 1 BC)
Surface Drip with Dynamic Wetting
From left to right
From the center
From right to left
Center Node: 0
Seepage Face with Specified Pressure Head
Pressure Head [cm]: -100
OK
Cancel
Help

Figure 111. The Special Boundary Conditions tab of the Boundary Condition Options dialog window.

6.3.3. *Triggered Irrigation*

Triggered Irrigation can be specified on the third tab of the **Boundary Condition Options** dialog window (Fig. 112). Irrigation can be triggered by a user-specified "**Pressure Head Triggering Irrigation**" (input) reached in the selected "**Observation Node Triggering Irrigation**". The irrigation starts after a user-specified **Lag Time** (input) at a user-specified **Irrigation Rate** or **Pressure Head** (input). The **Duration of Irrigation** has to be also specified.

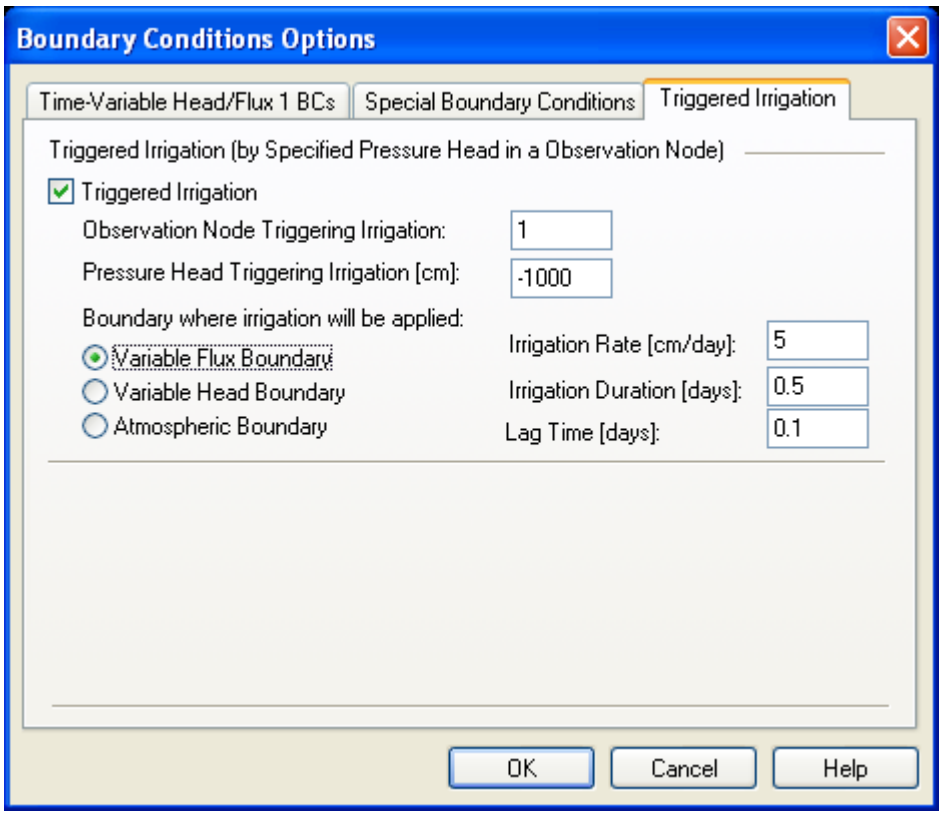


Figure 112. The Triggered Irrigation tab of the Boundary Condition Options dialog window.

Other parameters characterizing the flow domain (initial condition, material distribution) are defined in a similar way. Users must first select that part of the transport domain to which he/she wants to assign a particular value of the selected variable. It is possible to select the entire transport domain, part of it, or only individual nodes or elements. A particular part of the transport domain can be selected as follows: first move the mouse to a selected position. The beginning and end of the selection operation is framed by clicking the left mouse button. The selected area is the rectangle defined by the two mouse positions when the left mouse button was clicked. Selection can alternatively (instead of using the rectangular selection) be made using a rhomboid (with the *Edit->Select->Select by Rhomboid* command), circle (*Edit->Select->Select by Circle*) or polygon (*Edit->Select->Select by Polygon*). When the selection is completed, users must click the **Set values** button and specify the value of a particular variable. The given value will then be assigned to the selected area. When material numbers are to be specified, users can do this directly by clicking on the color representing a particular material (at the **Edit Bar**). All variables are assigned to nodal points, except for those defining anisotropy angles, the first and second components of anisotropy, and subregion numbers, which are all assigned to elements.

Scaling Factors can be generated for two-dimensional applications using a random generator by clicking on the command *Edit->Domain Properties->Stochastic Distribution of S.F.* that calls the **Stochastic Distribution of Scaling Factors** dialog window (Fig. 113). Each scaling factor can be generated either independently of the other scaling factors, or by assuming Miller-Miller similitude. In that case the program generates hydraulic conductivity scaling factors and automatically calculates from their values the pressure head scaling factors.

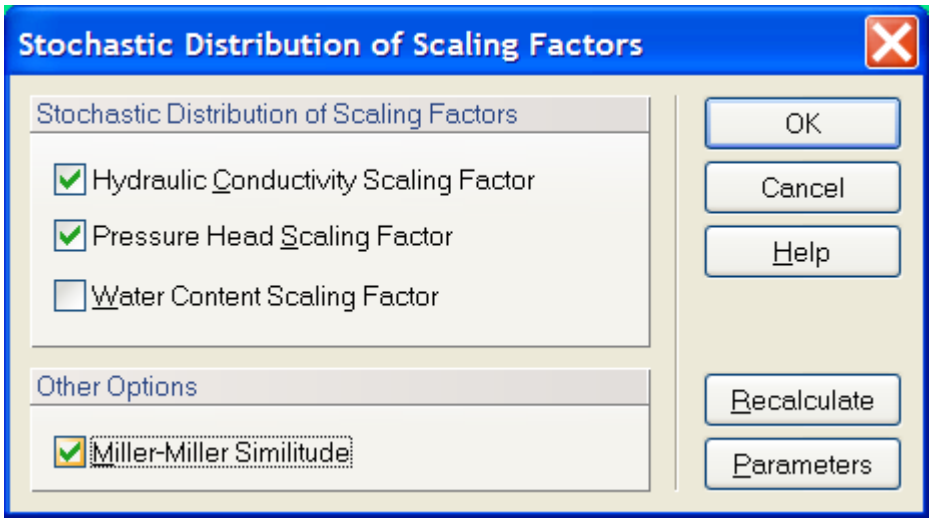


Figure 113. The Stochastic Distribution of Scaling Factors dialog window.

Parameters for random generation of the scaling factors are specified in the **Stochastic Parameters** dialog window (Fig. 114). In this dialog users need to specify whether the scaling

factors are normally or log-normally distributed using the check box *Log-Normal Distribution*), and provide values for the standard deviation of a particular scaling factor, and correlation lengths in the *x*- and *z*-directions (if the scaling factors are spatially correlated).

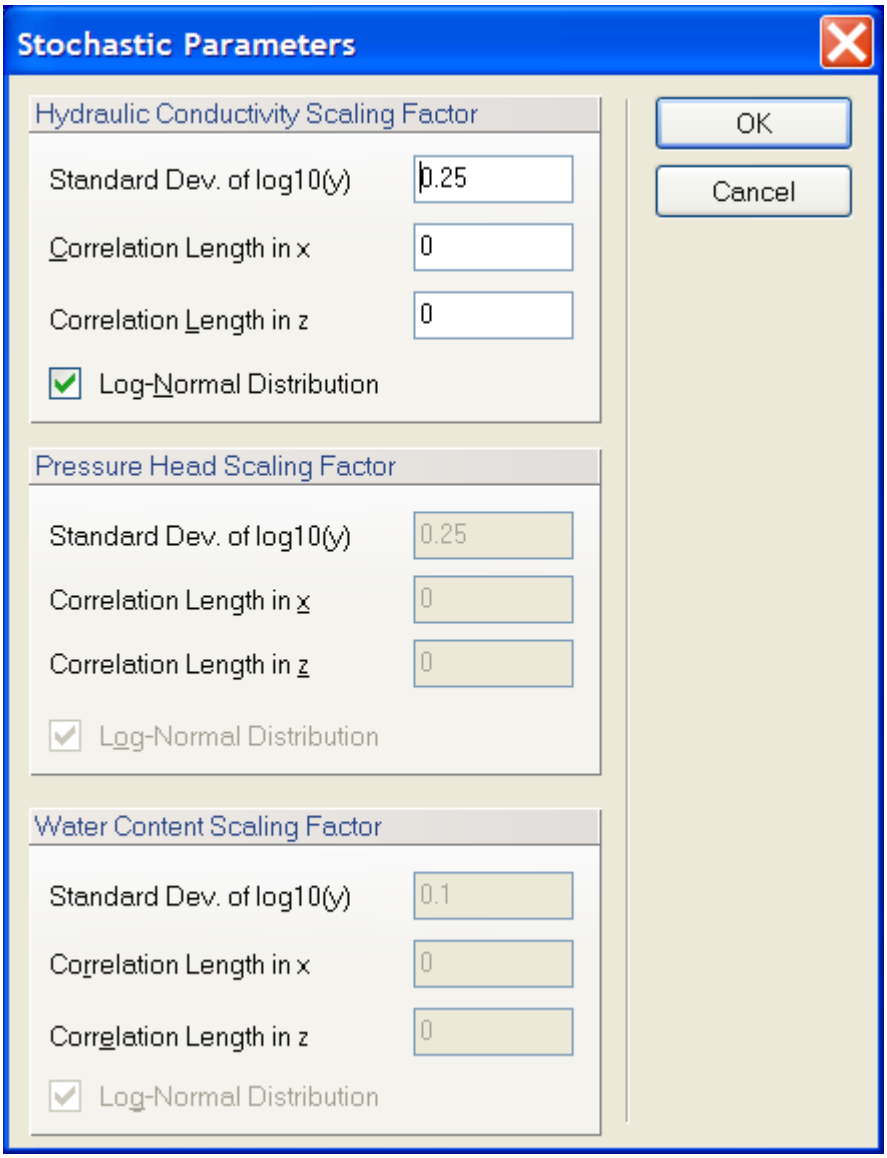


Figure 114. The Stochastic Parameters dialog window.

6.5. *Defining Properties on Geometrical Objects*

As described above, various spatially variable properties (e.g., material distribution, initial conditions, etc) can be specified in Version 2.0 of HYDRUS (Standard and Professional, not Lite) either:

a) directly on the **Finite Element Mesh** (FEM) (as done in Version 1.0), or
b) on **Geometrical Objects** (e.g., boundary curves, rectangles, circles, surfaces, solids) or **Geo Sections** (only in Version 2.0 and the Professional Version).

To be able to define properties on Geometrical Objects, one needs to first enable this option (Edit domain properties, initial and boundary conditions on Geometric Objects) in the **Domain Type and Units** dialog window (see Figs. 6 or 7).

Which option is used depends on the menu command *Edit->Properties and Conditions on FE-Mesh* (disabled when the FE-Mesh does not exist). A similar button switch is also available at the end of the tool bar ( ), next to the Results button, and at the **Edit Bar**.

However, to be able to use this option (to specify properties on **Geo Sections**), the Transport Domain must be defined using (or divided into) a set of **Geometrical Objects**, on which various properties can then be specified. An example of the transport domain divided onto three components (or **Surfaces**) S2, S2, or S3 is shown in Figure 115.

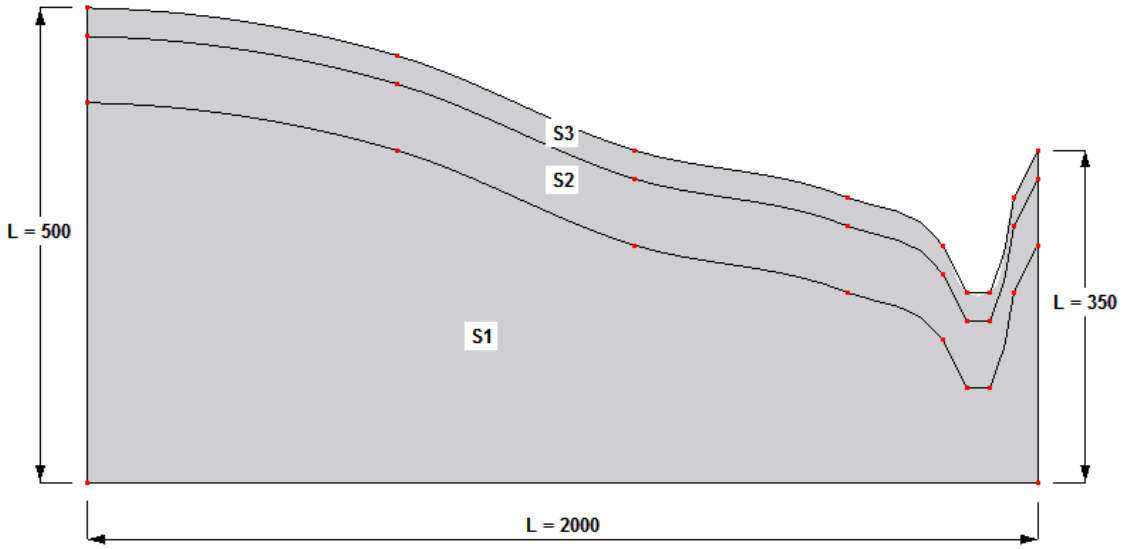


Figure 115. An example of the transport domain defined using three components S1, S2, and S3.

While for two-dimensional problems the **Geo Sections** (displayed at the **Navigator Bar** at the **Section Tab**) need to be defined manually, for three-dimensional problems they can also be generated automatically (see Section 8.1.8 what and how are these **Sections** generated). At the same time when HYDRUS generates 3D objects, it also generates **Surfaces** belonging to each of

these objects. Some of these **Surfaces** are *Horizontal* and some are *Vertical* (although these terms are only approximate). **Surfaces** can then be used to specify **Boundary Conditions**.

Vertical Surfaces are always created over the entire curve, which forms the boundary of the **Base Surface**. When the boundary of the **Base Surface** consists of several curves, then an independent *Vertical* **Surface** is created above each curve. Since the curves of the **Base Surface** can be arbitrarily divided, *Vertical Surfaces* can be created relatively freely.

While the text above in Section 6 refers to the first approach (specifying properties at FE-Mesh), the second approach (on Geo Objects) is briefly described below. While this latter approach can be used for all Domain Properties, and Initial and Boundary Conditions, we will demonstrate its use below on Material Distribution, for which it seems to be the most relevant. There are multiple commands that are common for most properties when defining Domain Properties, Boundary Conditions, and Initial Conditions on Geometrical Objects. These commands are listed in the *Commands* part of the **Edit Bar** and are listed in Table 20.

Table 20. Definition of commands used to manipulate Property Objects.

Command	**Description**
New Property*	Creates a new Property Object. For some Properties, there is a list of available options and user needs to select from this list (e.g., water flow boundary conditions) or can extend this list (e.g., Materials). For others, user needs to define values (e.g., scaling factors) or functional forms (e.g., initial conditions) of new Property Objects.
Set Property	Selects one particular Property from a list or Property Objects and assigns it to a selected Geo Object(s).
Clear Property	Clears a particular Property from selected Geometrical Points. This command is used only for Properties that do not have a default Property (e.g., Nodal Recharge, Observation Nodes).
Clear All Properties	Clears all assigned Properties from geometrical objects and assigns default properties where required (e.g., Materials) to the entire transport domain. Note that this command does not delete definitions of Properties (as done by the Delete All Properties command), which thus remain available in the data tree of the Navigator Bar.
Delete Property	Deletes a Property Object selected in the data tree of the Navigator Bar. This command is not used for Materials or Subregions, the number of which is specified elsewhere.
Delete All Properties	Deletes all Property Objects defined for a particular Property, except for a default Property (which is defined for those Properties where a default Property is needed). Similarly as for the Delete Property commands, this command does not exist for Materials and Subregions.

Sort Properties	Calls a dialog window "Sort Property Objects", which displays all available Property Objects. Here, (the sequence of) the Property Objects can be arbitrarily rearranged.
Transfer to FE-Mesh	Transfers information about a particular Property defined on Geo Objects to the FE-Mesh. Note that this command is available only when information about a particular Property on Geo Objects and FE-Mesh does not correspond. This can occur, for example, when Property is defined (or refined) on FE-Mesh.
Edit Property	Recalls a dialog window with parameters of a particular Property to edit.

---

*Note that the word Property is used in place of a particular Property Object, such as Domain Property (e.g., Material, Observation Node), Boundary Condition, or Initial Condition.

6.5.1. *Materials on Geometrical Objects*

Let's assign three different materials to three **Surfaces** in Figure 115. When only one material is defined (which is a default option in each new project), one needs to first define multiple materials (and/or their soil hydraulic properties). This can be done as usual using the Menu command *Edit->Flow and Transport Parameters->Water Flow Parameters->Soil Hydraulic Parameters*. The same dialog window (Fig. 19) can be also displayed by clicking on the **New Material** or **Edit Materials** commands on the **Edit Bar** (Fig. 116). Note that in Version 2.0 of HYDRUS, one can name materials.

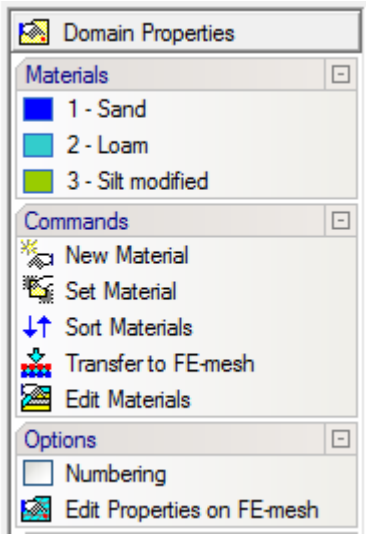


Figure 116. The upper part of the Edit Bar, which displays defined materials and commands for various actions with materials.

There are three different ways of assigning materials to particular geometrical objects (**Surfaces**):

a) Click on a particular **Surface** (Geo Object) (to select it) and then on a **Material** (1, 2, or 3) in the **Materials** section of the **Edit Bar** to assign it.
b) Click on a Material (1, 2, or 3) in the **Materials** section (to select it) of the **Edit Bar** and then on a particular **Surface** (to assign it).
c) Click on the command **Set Material** in the **Commands** section of the **Edit Bar**, from the list box of the **Set Materials** window (Fig. 117) **Select Material to set**, click Assign to close the window, and click on a particular **Surface** to assign the selected material.

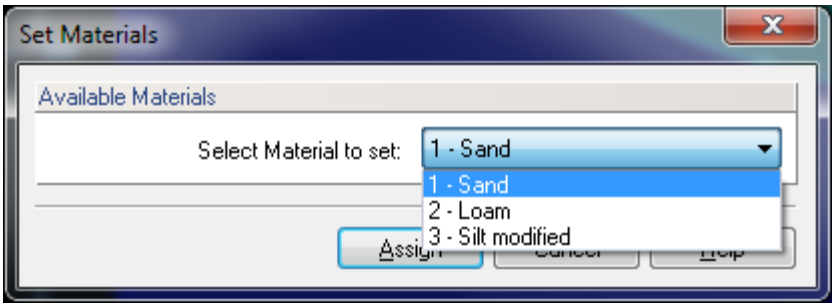


Figure 117. The Set Materials dialog window.

Note that nodes that are at the curve shared by two surfaces will be assigned a material with a higher number. Color squares at nodes defining the **Geometry** (Fig. 118) indicate, which material will be assigned to curves shared by two **Surfaces**.

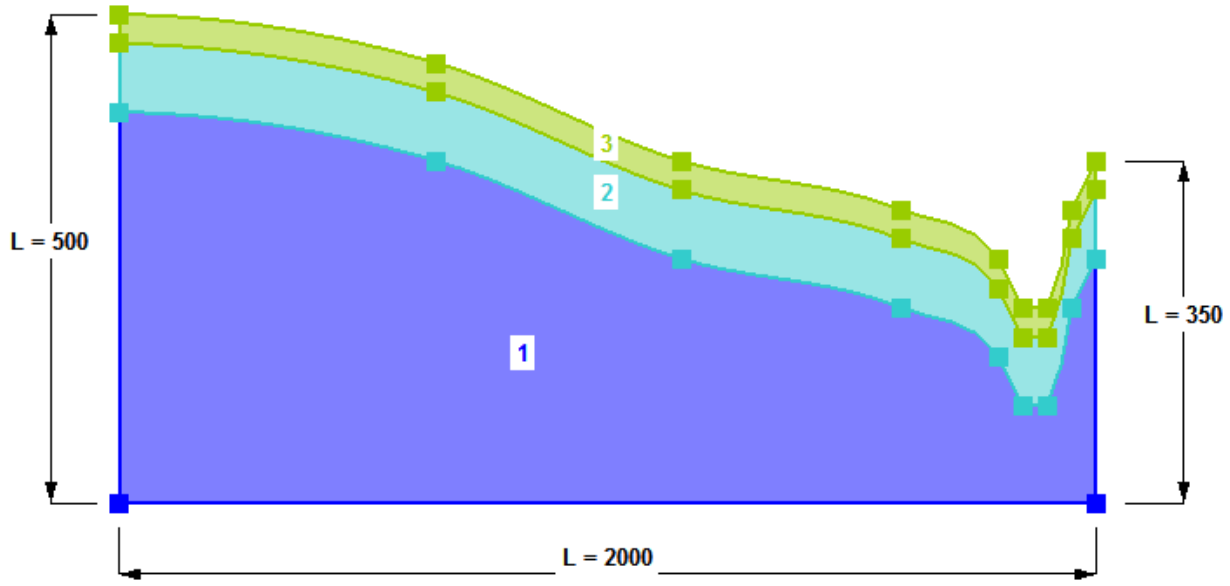


Figure 118. The transport domain with materials specified on geometrical objects.

The sequence of materials (as well as other objects, such as Initial Conditions) can be reordered or sorted using the **Sort Materials** command on the **Edit Bar** and the **Sort Property Objects** dialog window (Fig. 119). In this dialog, the order of materials can be sorted using the **Top**, **Up**,

Down, and **Bottom** command. While the sequence of materials can be sorted, colors representing the first, second, and other materials will remain the same.

Sorting can be done in two modes. When the **Auto-apply** check box is checked, any change done in the **Sort Property Object** window is immediately transferred to the transport domain and to the rest of the program. When this checkbox is unchecked, changes made in this dialog are transferred to the rest of the program only when the **Apply** command is clicked or after the window is closed using the **OK** button.

The command **Renumber All** can be used to renumber the **Property Objects**. This is useful, when some previously defined Properties were deleted and the numbering is no longer sequential.

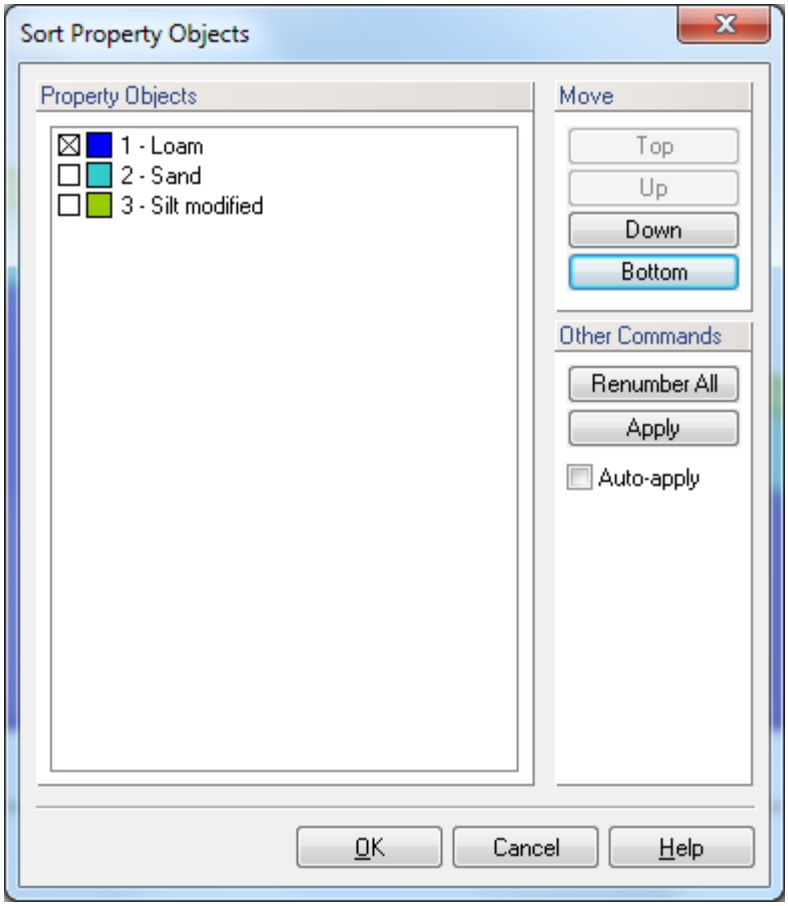


Figure 119. The Sort Property Objects dialog window.

A single click on any **Surface** will select this surface. A double click on any **Surface** will open a dialog for a Property assigned to a particular surface that is currently displayed, e.g., the **Edit Materials** dialog window (Fig. 120). In this dialog, one can change the **Name** of the material, its **Color** (the **Default** check box indicates whether the Color has been changed), **Assign** it **to** different **Surfaces** (indicated by their numbers), and register brief **Remarks** characterizing a particular material.

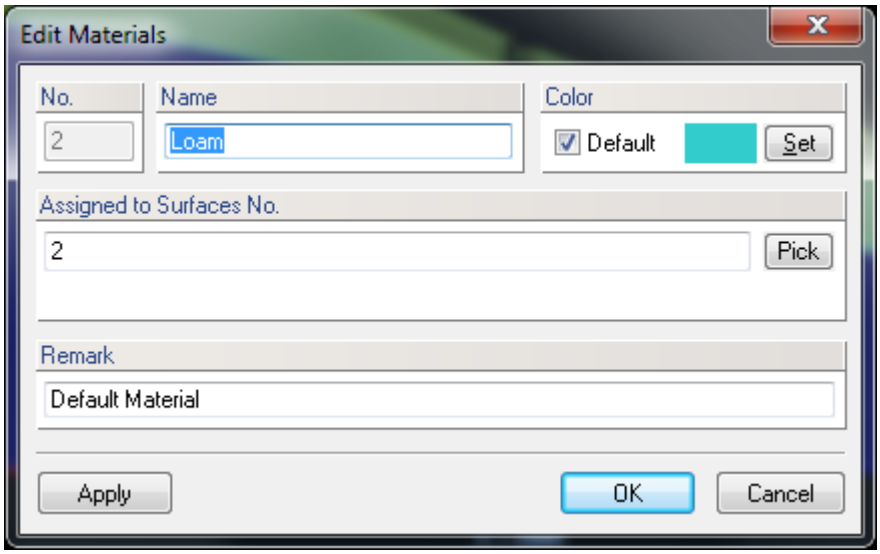
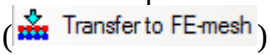


Figure 120. The Edit Materials dialog window.

Once the FE-Mesh exists, assigned properties (e.g., Materials) can be transferred on the FE Nodes (if it exist) using the **Edit Properties on FE-Mesh** (when FEM exists and a particular Property has not been yet edited on FEM) or the **Transfer to FE-Mesh** (

) (when a particular Property has already been edited on FEM) commands located on the **Edit Bar** (Fig. 116). Here the assignment of materials can be further edited, refined, and finalized. However, these changes cannot be transferred back on the **Geometrical Objects**. After changes have been made on FEM and thus Properties assigned on FEM and Geo Objects no longer correspond, the command **Transfer to FE-Mesh** can be used to synchronize again the information in the two modes (from Geometrical Objects to FEM).

The **Edit Bar** commands **Edit Properties on FE-Mesh** and **Edit Properties on Geo Objects** switches from one way of assigning properties (on Geo Objects) to another (on FEM).

Similar approach and similar commands can be used to assign other Domain Properties, and Initial and Boundary Conditions.

6.5.2. *Observation Nodes on Geometrical Objects*

Observation Nodes are entered on Geometrical Objects using either the Menu command *Insert->Domain Properties->Observation Nodes* or the **New Observation Node** command on the **Edit Bar**. The **New Observation Node** command can be used in the **Edit Properties on Geo Objects** mode to define observation nodes only on **Points** defining the **Geometry** (i.e., Points defining boundary curves). Observation nodes for any other location have to be specified on the FE-Mesh directly. The same is true also for Drains and Flowing Particles.

The **Edit Observation Node** window (Fig. 121) is displayed when double-clicking on an observation node in the **View** window (when working in the Properties on Geometrical Objects mode) or an Observation Node item in the **Navigator Bar**. This window displays

a) the **Name** of the observation node (note that the observation node can be renamed using a brief text, such as drain, tensiometer, TDR, etc),
b) indication whether it is **Defined at Geometrical Node** or **FE-Mesh Node**, and
c) a brief **Remark** (note).

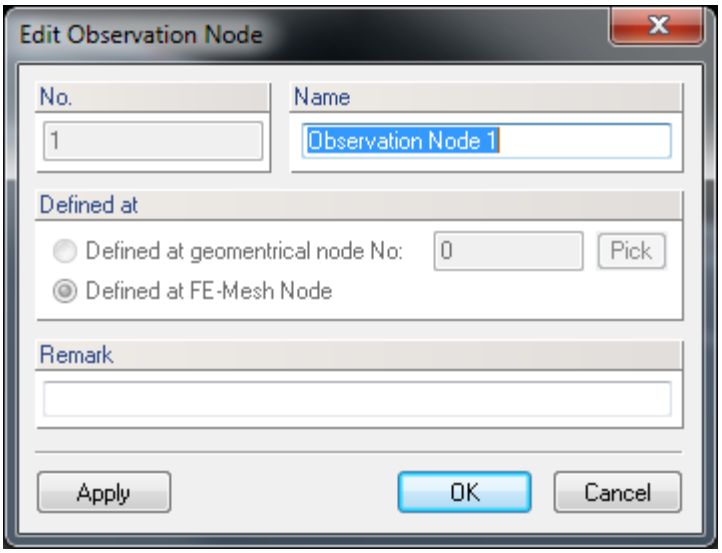


Figure 121. The Observation Node dialog window.

6.5.3. *Initial Conditions at Geometrical Objects*

Property Objects for Initial Conditions are defined or edited using the **New** or **Edit Pressure Head** (**Concentration**) **Initial Condition** dialog windows shown in Figure 122. Note that parameters and values that are entered in these dialogs are the same as those entered in Figure 107, when defining Initial Conditions directly at the FE-Mesh. Here, one can additionally define the **Name** of the Initial Condition, the **Color** which represents it (either **Default** or selected), register a brief **Remark**, and select to which surfaces it is assigned to (**Assigned to Surfaces No:**).

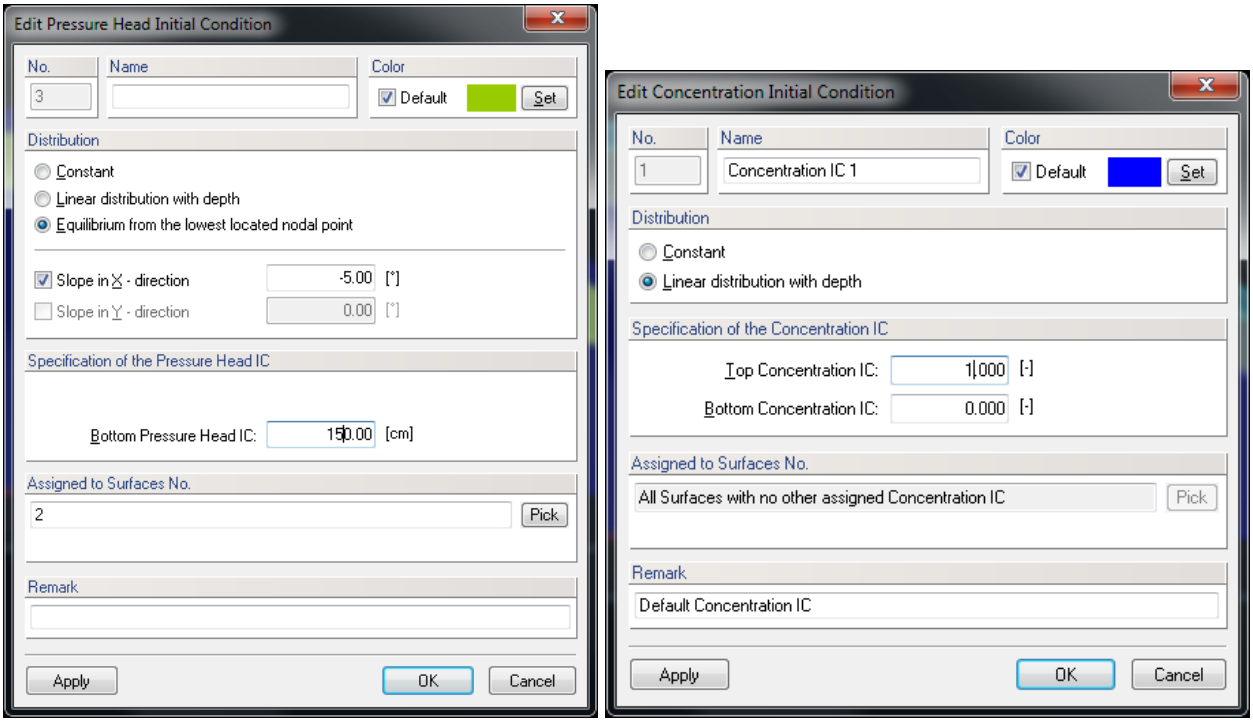


Figure 122. The Edit Pressure Head (left) and Concentration (right) Initial Conditions dialog window.

6.5.4. *Boundary Conditions at Geometrical Objects*

New Property Objects for Boundary Conditions must be selected from existing boundary conditions used in HYDRUS. For example, for Water Flow Boundary Conditions, new Objects are selected from the list box **Boundary Condition Type** displayed in Figure 123. Similarly as for other Properties, in this dialog one can define **Name**, **Color**, register a **Remark**, assigned Boundary Condition at selected Boundary Curves, and, if needed, specify required parameters (e.g., for Deep Drainage BC).

Notes:

1. When the same pressure head initial (or boundary) condition involving either "Equilibrium from the lowest located point" or "A linear distribution" is chosen for multiple surfaces (or curves), then this condition is applied globally to all selected surfaces (e.g., a single point with the lowest z-coordinate is found for all selected surfaces).
2. The default solute and heat transport boundary conditions are the **Third-Type BC**s, which are listed right after the **No Flux** BC. This BC is by default assigned to all boundaries, to which the water flow BCs have been defined. Note that if you redefine this BC (e.g., change the Third-Type BC into the First-Type BC), the newly defined BC will be used as a default BC for solute and or heat transport.

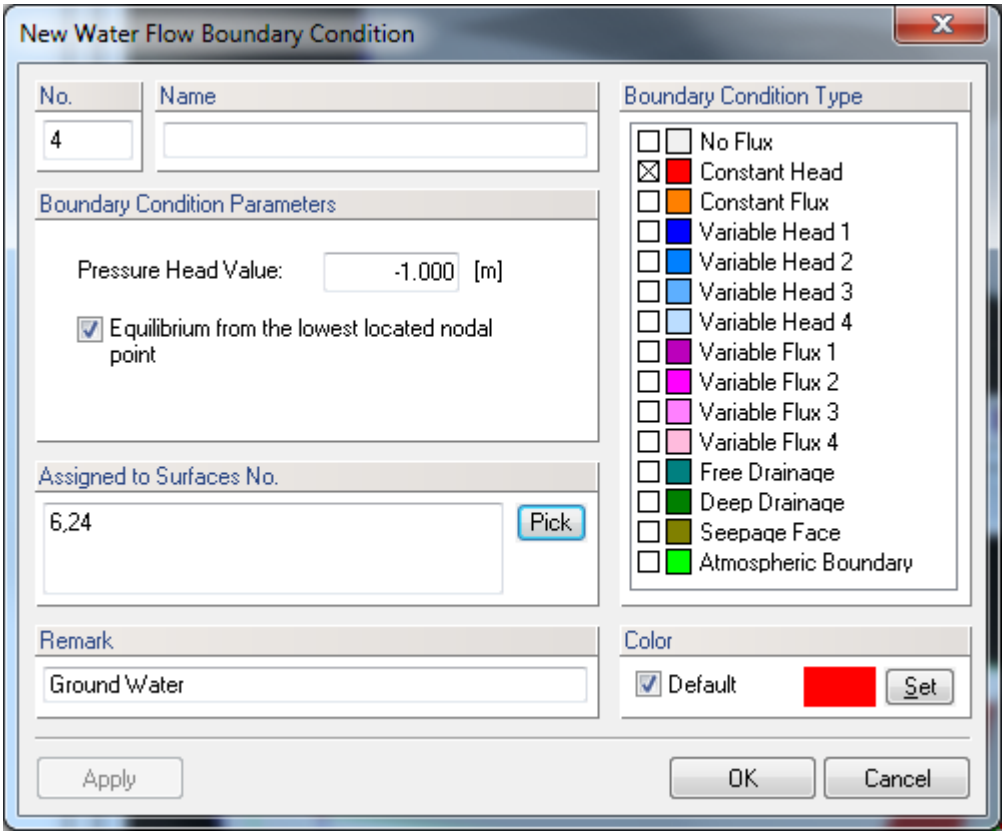


Figure 123. The Edit Water Flow Boundary Condition dialog window.

6.5.5. Additional Notes on Properties at Geometrical Objects

a) When the same pressure head initial (or boundary) condition involving either "Equilibrium from the lowest located point" or "A linear distribution" is chosen for multiple surfaces (or curves), then this condition is applied globally to all selected surfaces (e.g., a single point with the lowest z-coordinate is found for all selected surfaces).
b) Nodes that are at the boundary line shared by two surfaces (or at the surface shared by two volumes) are assigned the property value with a higher number. The sequence in the list of properties can be adjusted using the command **Sort Property** (where Property is either Material, Scaling Factor, etc) at the **Edit Bar** (Fig. 119).
c) The option to assign Properties at Geometrical Objects is not available for simple parametric (i.e., **Rectangular** or **Hexahedral**) Geometries available in the Lite Version of HYDRUS.
d) **Name**: One can provide a **Name** for each newly defined **Property Object**. When user does not define a **Name** for a **Property Object**, the GUI will automatically generate a generic name that is then used throughout the project (e.g., on the **Navigator** and **Edit Bars**).

7. Graphical Output

Graphical output is divided into two main parts. In the first part, variables which change spatially throughout the transport domain are displayed by means of contour maps, isolines, isosurfaces, or isobands (**Results – Graphical Display** on the **Data Tab** of the **Navigator Bar**, or *Options->Graph Type*). Additional information such as boundary fluxes and/or soil hydraulic properties are displayed using *x-y* graphs (**Results – Other Information** on the **Data Tab** of the **Navigator Bar**, or using the **Results Menu**).

7.1. *Results – Graphical Display*

Results of a simulation can be displayed by means of contour maps, isolines, isobands, isosurfaces, color points, color edges, spectral maps, and/or velocity vectors (*Graph Type* at the **View Tab** of the **Navigator Bar** or *Options->Graph Type->Isolines*), and/or by animation using both contour and spectral maps. The number of colors in the color spectrum, as well as the numerical increment between isolines, can be selected using the **Edit Isoband Value and Color Spectra** dialog window (Fig. 127). Contour and spectral maps may be drawn for the pressure head, water content, temperature, solute concentration (in the equilibrium or nonequilibrium phase), and/or velocity. Animation of these four variables is also possible (*Flow Animation* on the *Results* version of the **Edit Bar**, or using *Results->Time Layer->Animation*). Graphs of all variables along the boundaries (*Boundary-Line Chart* on the *Results* version of the **Edit Bar**, or using *Results->Charts->Boundary Line*), as well as those along any selected cross-section (*Cross-Section Chart* on the *Results* version of the **Edit Bar** or *Results->Charts->Cross-Section*) can be readily obtained.

The entire finite element mesh, the boundary nodes, and the numbering of nodes, elements and/or edges, can be displayed also (using the **Display Options** dialog window (Fig. 126), or *Options->Display Options->Edit*), together with isolines and spectral graphs. Users may zoom into a certain part of the transport domain, and can enlarge or reduce the transport domain, among other features.

Flow animation is an alternative to displaying results at one particular time. Distributions during flow animation are displayed continuously at consecutive times, thereby visualizing the flow and transport process. Note, however, that display times are defined by the print time intervals specified in the input data file. This means that the print times must be at constant intervals so that the time scale of the flow animation will not be distorted. In other words, undistorted flow animation requires that the print time intervals be constant. The speed of the flow animation depends on the hardware being used, i.e., the speed of the microprocessor and graphical card.

7.1.1. *Displayed Variables*

Multiple variables can be displayed in the View window. A comprehensive list of standard and alternative variables that can be displayed in the View window are summarized in Tables 21 and 22, respectively.

Table 21. Standard variables displayed in the View Window of the Results tab (Results - Graphical Display).

Variable	Description
Pressure Head	Pressure head h [L]; displayed always
Water Content	Water content θ [-] (or θ_m when dual-porosity model is used); displayed always
Velocity	Values of the Darcy's flux q [LT^{-1}]; displayed always
Velocity Vectors	Darcy's flux vectors q [LT^{-1}]; displayed always
Root Water Uptake	Root water uptake S [T^{-1}]; displayed when root water uptake is considered
Concentration *i*	Liquid phase concentration c [$M_cL_w^{-3}$]; displayed when solute transport in the standard module is simulated.
Sorbed Noneq. Conc. *i*	Concentration of kinetically sorbed solute s^k [$M_cM_s^{-1}$]$^+$; displayed when solute transport in the standard module is simulated and when the two-site sorption model is considered.
Immobile Conc. *i*	Concentration in the immobile water c_{im} [$M_cL_w^{-3}$]; displayed when solute transport in the standard module is simulated and mobile-immobile water or dual-porosity models are considered.
Temperature	Temperature T [^oC]; displayed when heat transport is simulated.
Unsatchem Variables	Major ions (Ca, Mg, Na, K, HCO3, SO4, Cl, tracer, sorbed Ca, sorbed Mg, sorbed Na, sorbed K, calcite, gypsum, dolomite, nesquohonite, hydromagnesite, sepiolite; displayed when the Unsatchem module is used.
Wetland Variables	Various variables used in the two constructed wetlands modules CW2D and CWM1 (see the Wetlands module manual for details).

$^+$ Subscripts *c*, *s*, and *w* refer to contaminant, soil, and water.

Table 22. Alternative variables that can be displayed in the View Window of the Results tab.

Variable	Description
Pressure Head	Standard display
Total Pressure Head	Total Pressure Head H (=h+z) [L]; alternative display
Water Content	Standard display
Mobile Water Content	Water content in the mobile phase θ or θ_m [-]; default display
Immobile Water Content	Water content in the immobile phase q_{im} [-]; displayed when dual-porosity model is used.
Total Water Content	Total water content θ (=θ_m+θ_{im}); displayed when dual-porosity model is used.
Velocity	Standard display
Total Value	Darcy's flux [LT^{-1}]; default display
x-component	x-component of the Darcy's flux q [LT^{-1}]
y-component	y-component of the Darcy's flux q [LT^{-1}]
z-component	z-component of the Darcy's flux q [LT^{-1}]
Concentration Options	
Liquid Equil. Phase Conc.	Liquid phase concentration c [$M_cL_w^{-3}$]$^+$; default display.
Sorbed Equilibrium Conc.	Concentration of instantaneously sorbed solute s^e [$M_cM_s^{-1}$].
Sorbed Total Concentration	Sorbed concentration s= s^e + s^k [$M_cM_s^{-1}$].
Gas Phase Concentration	Gas phase concentration g (=K_Hc) [$M_cL_a^{-3}$]
Total Concentration	Total concentration mass S [$M_cL_s^{-3}$]
Sorbed Concentration Options	
Sorption Sites 1	Sorbed concentration on first kinetic sorption sites s_1^k [$M_cM_s^{-1}$]
Sorption Sites 2	Sorbed concentration on second kinetic sorption sites s_2^k [$M_cM_s^{-1}$]
Total Sorbed Conc.	Total sorbed concentration $s^k = s_1^k + s_2^k$ [$M_cM_s^{-1}$]

$^+$ Subscripts c, s, a, and w refer to contaminant, soil, air, and water.

Table 23. Definition of various concentration modes (for linear sorption model).

	Equilibrium model	Mobile-immobile model	Two-site sorption model	Two-kinetic sites model
Sorbed Equilibrium Concentration $[M_c M_s^{-1}]$	$K_D c$	$K_D f c_m$	$f_e K_D c$	$K_D c$
Sorbed Nonequil. Concentration $[M_c M_s^{-1}]$	-	$K_D(1-f)c_{im}$	s^k	$s_1^k + s_2^k$
Sorbed Total Concentration $[M_c M_s^{-1}]$	$K_D c$	$K_D\left[f c_m + (1-f)c_{im}\right]$	$f_e K_D c + s^k$	$K_D c + s_1^k + s_2^k$
Gas phase concentration $[M_c L_a^{-3}]$	$K_H c$	$K_H c$	$K_H c$	$K_H c$
Solute mass in the liquid phase, S_l $[M_c L_s^{-3}]$	$c\theta$	$c_m\theta_m + c_{im}\theta_{im}$	$c\theta$	$c\theta$
Solute mass in the solid phase, S_s $[M_c L_s^{-3}]$	$\rho K_D c$	$\rho K_D\left[f c_m + (1-f)c_{im}\right]$	$\rho\left(f_e K_D c + s^k\right)$	$\rho\left(s_1^k + s_2^k\right)$
Solute mass in the gas phase, S_g $[M_c L_s^{-3}]$	$K_H c a$	$K_H c a$	$K_H c a$	$K_H c a$
Total Concentration, S $[M_c L_s^{-3}]$	$S_l+S_s+S_g$	$S_l+S_s+S_g$	$S_l+S_s+S_g$	$S_l+S_s+S_g$

a air content $[L_a^3 L_s^{-3}]$

c liquid phase concentration $[M_c L_w^{-3}]$

c_m liquid phase concentration in the mobile phase $[M_c L_w^{-3}]$

c_{im} liquid phase concentration in the immobile phase $[M_c L_w^{-3}]$

θ water content $[L_w^3 L_s^{-3}]$

θ_m water content in the mobile phase $[L_w^3 L_s^{-3}]$

θ_{im} water content in the immobile phase $[L_w^3 L_s^{-3}]$

K_D distribution (sorption) coefficient $[L_w^3 M_s^{-1}]$

K_H Henry's law constant [-]

S_l solute mass in the liquid phase $[M_c L_s^{-3}]$

S_s solute mass in the solid phase $[M_c L_s^{-3}]$

S_g solute mass in the gas phase $[M_c L_s^{-3}]$

S total concentration (solute mass), $S=S_l+S_s+S_g$ $[M_c L_s^{-3}]$

s solid phase concentration $[M_c M_s^{-1}]$

s^k solid phase concentration on kinetic sorption sites $[M_c M_s^{-1}]$

s_1^k solid phase concentration on first kinetic sorption sites $[M_c M_s^{-1}]$

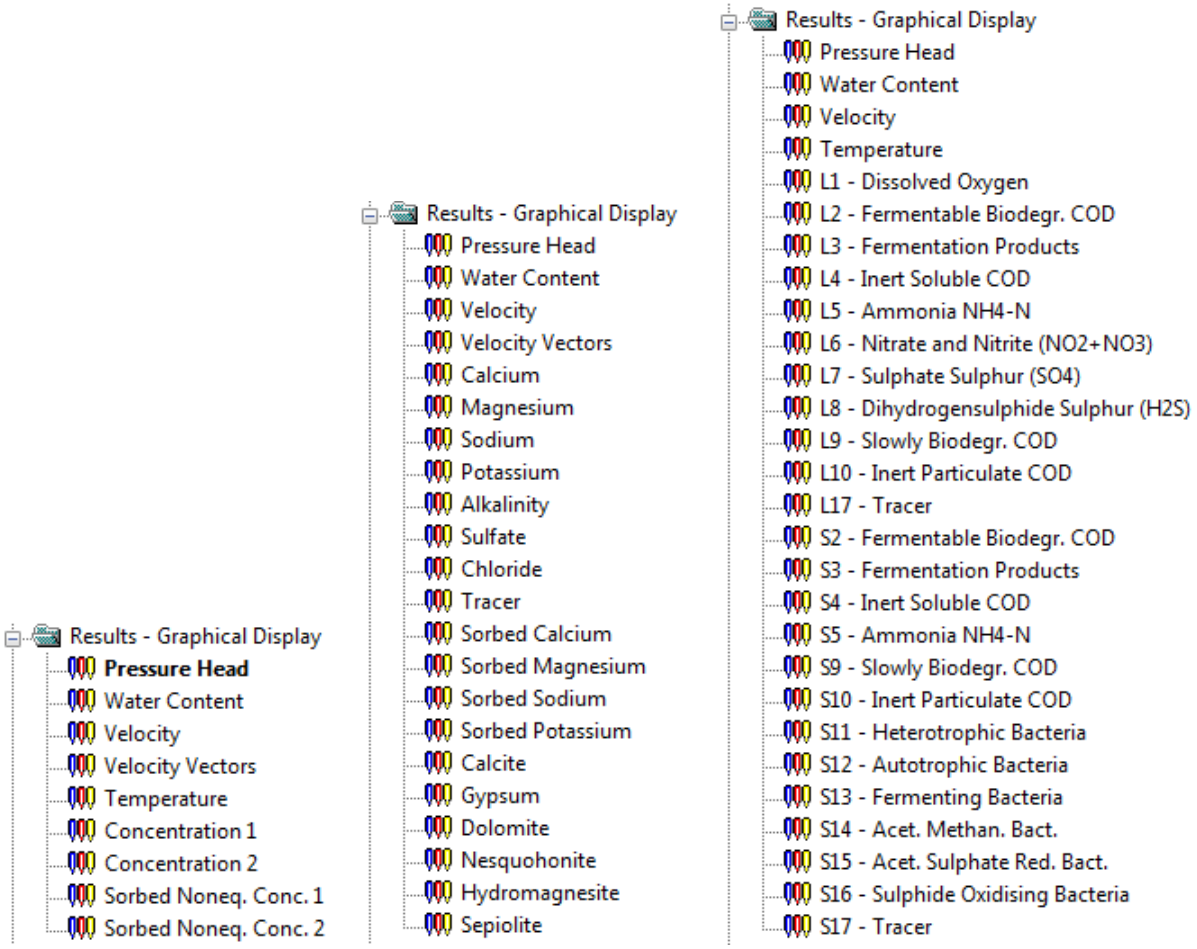


Figure 124. The "Results - Graphical Display" part of Data Tab of the Navigator Bar for the standard (left), Unsatchem (centre), and Wetland (right) modules.

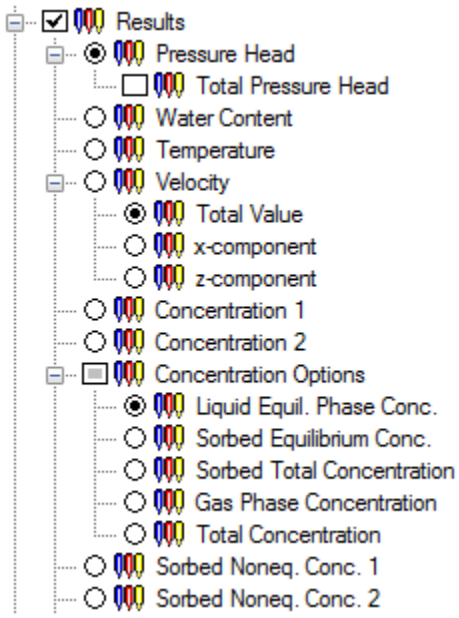


Figure 125. The "Results" part of the View Tab of the Navigator Bar with the display of various alternative variables.

7.1.2. *Display Options*

The **Display Options** dialog window (Fig. 126) allows users to select

a) how different objects from the **Category** list are to be displayed,
b) what **colors** are to be used (colors can be redefined by clicking on the *Edit Color* command button),
c) whether **lines** are displayed as solid, dotted, dashed or dash-dotted (*Line Type*), and what *Thickness* should be used, and
d) the position of **numbers** for various types of *numberings*, fonts for the numbers, and whether or not numbers are *Transparent*.

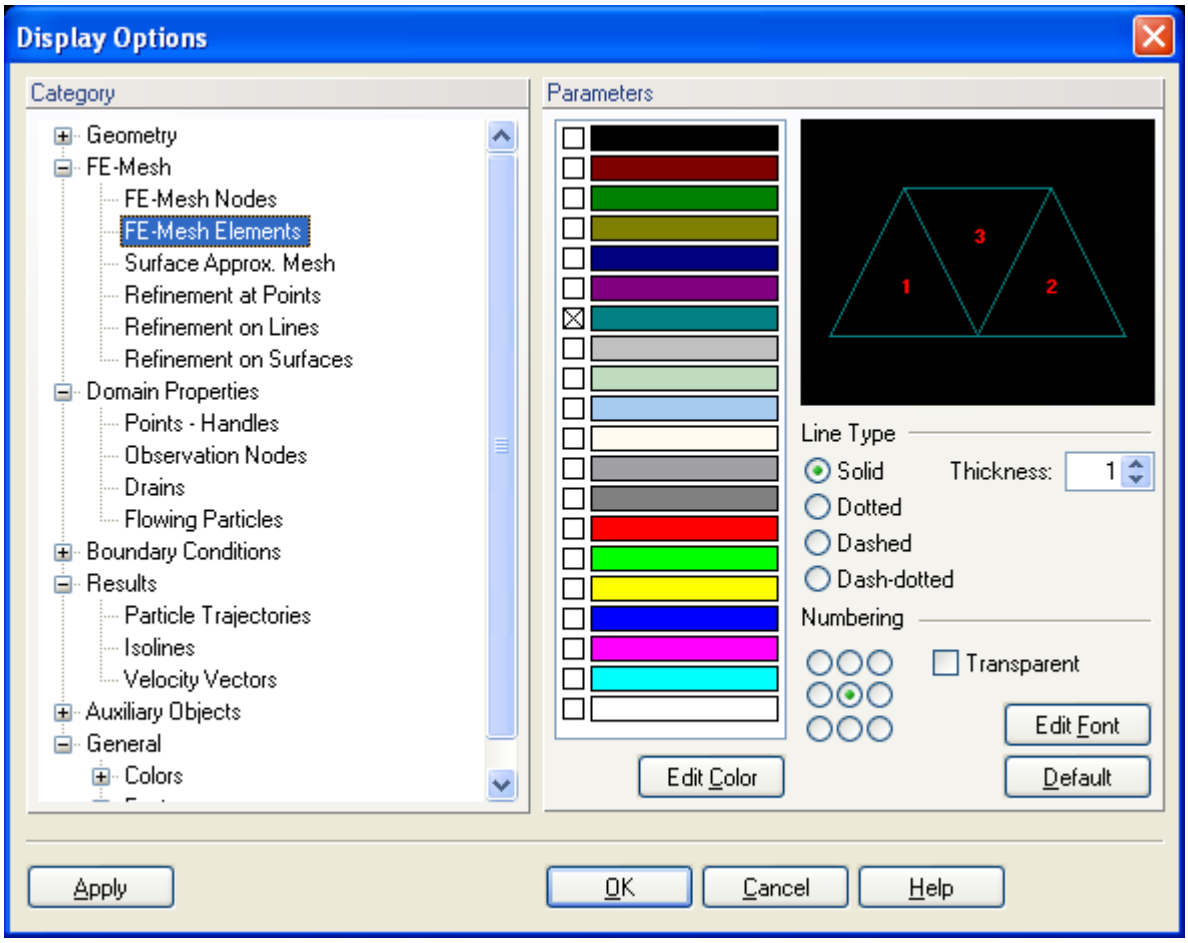


Figure 126. The Display Options dialog window.

7.1.3. *Edit Isoband Value and Color Spectra*

The **Edit Isoband Value and Color Spectra** dialog window (Fig. 127) (called by left-clicking the color scale display options of the **Results** version of the **Edit Bar**) allows users to define colors for display of isobands isosurfaces, and color spectra, and values of particular isolines. The default scale has always 11 values, which corresponds to 11 colors for color contours and 12 colors for isolines. Values at the scale are calculated by evenly dividing the interval between the minimum and maximum of a particular variable. Numbers are formatted depending on units used to display a particular variable. When the number of displayed digits is insufficient, it is possible to use a scientific format (**E-format**). The E-format is then used also on the Edit Bar and for printing (only for a particular variable).

Note that switching from a regular format to the **E-format** represents also switching from the **Standard Scale** to the **Custom Scale** (see below), which is then kept for the display of the same variable at other times. Returning to the **Standard Scale** may be required to adjust the scale as needed to display a given variable at the new time.

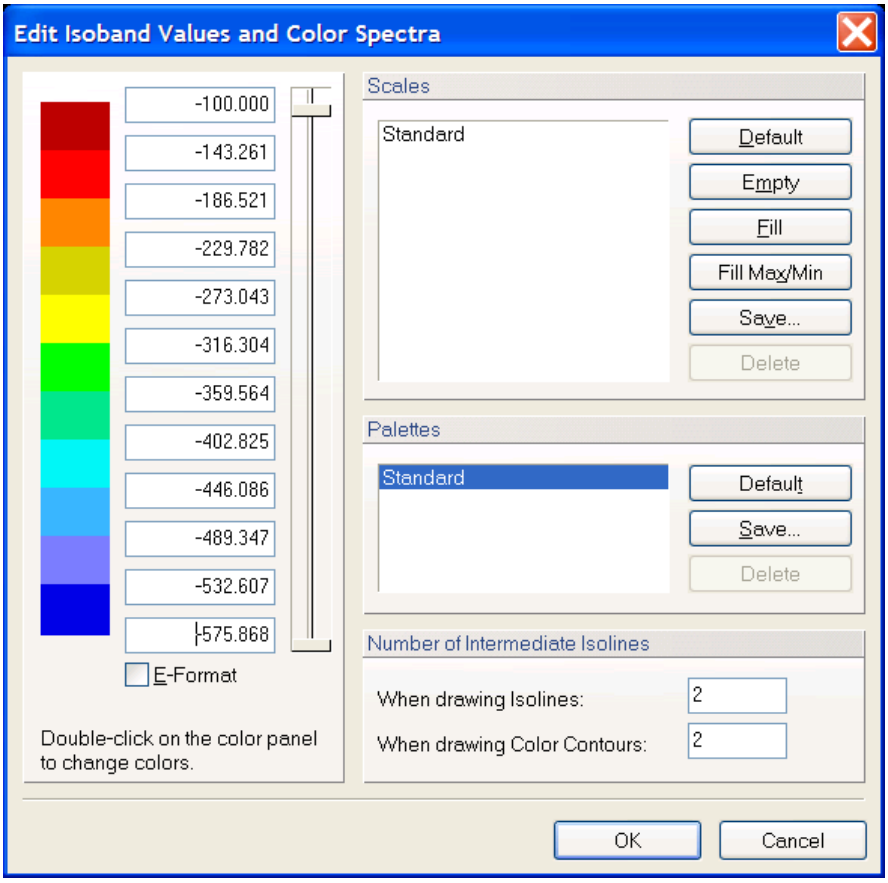


Figure 127. The Edit Isoband Value and Color Spectra dialog window.

Users can also define the **Isoline scales**. This can be done by simply changing numbers in the edit boxes next to the colors. If the numbers are not in an increasing or decreasing order, a

warning will be issued. Newly created **Isoline scales** can be saved (again locally or globally) and used later. Users need to specify only the maximum and minimum values (the top and bottom edit boxes); after clicking the **Fill** command, the program will calculate and fill (complete) the intermediate numbers by interpolation. A specified **Number of Intermediate Isolines** can be drawn between the main isolines using *When drawing Isolines* or *When drawing Color Contours*. This number is by default equal to zero. Five intermediate isolines are used in Figure 128.

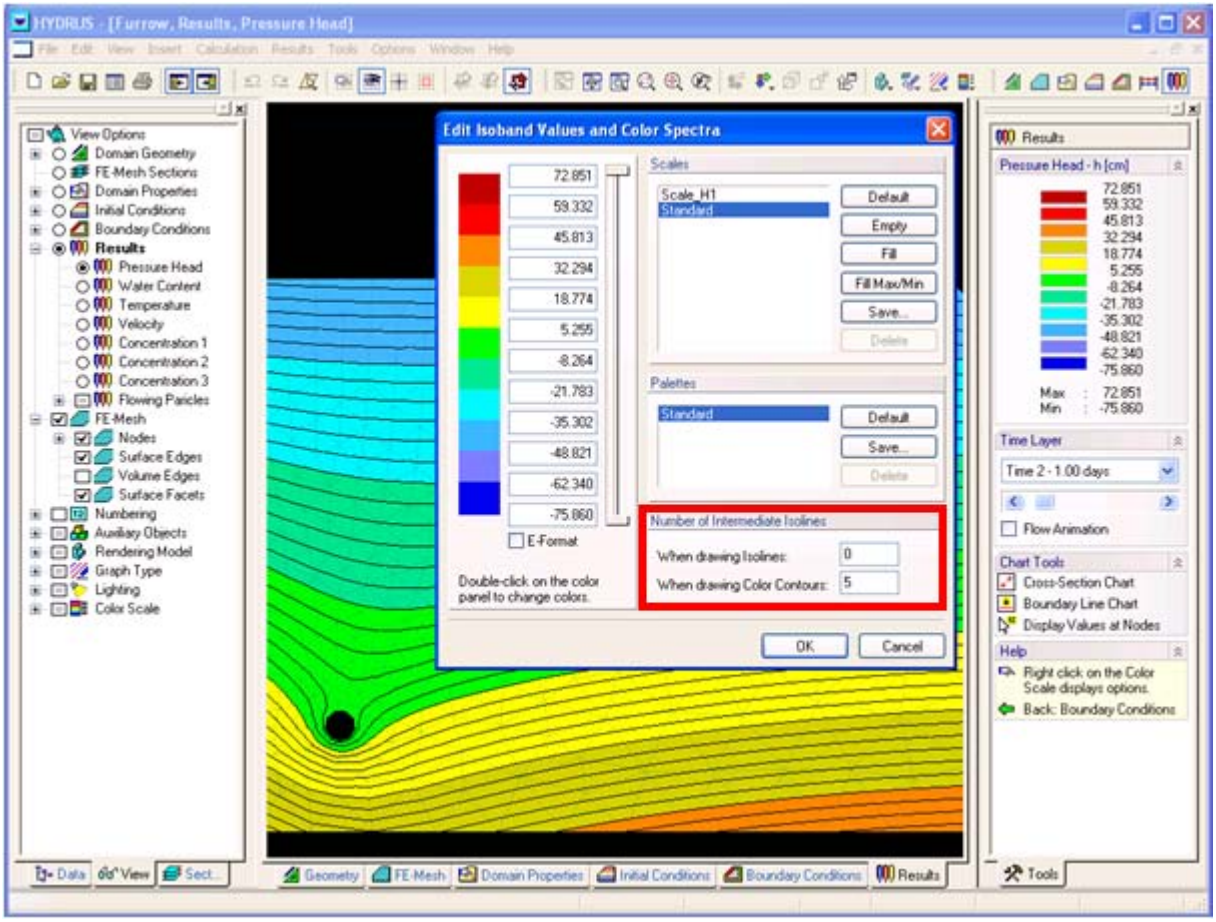


Figure 128. The use of intermediate isolines.

Minimum and maximum numbers of the scale are automatically adjusted to a particular problem and for a particular variable. By default, HYDRUS searches all output time levels of a particular project for the minimum and maximum values of a particular variable, and then leaves the scale invariant in time between these two values. The scale, however, can also be automatically adjusted for each time level by specifying the minimum and maximum values for a particular variable and a particular print time when the option *Min/Max glob. in time* from the **Color Scale View Options** of the **View Tab** of the **Navigator Bar** is deselected. Similarly, the scale can be automatically adjusted for a particular layer of the FE-mesh (a section) (the minimum and maximum values for a particular variable and a particular section) when the option *Min/Max glob. in space* from the **Color Scale View Options** of the **View Tab** of the **Navigator Bar** is unselected.

After clicking on the color panel with the **left** mouse button, the **Color** dialog window (Fig. 129) appears, in which one can redefine colors to be used in displays. By default a **Standard Palette** is used. If a Custom Scale exists for a displayed variable, colors for this scale will be displayed even when **Standard Scale** was currently used (since the Standard Scale can not be edited). Palettes with newly defined colors can be saved (Save Palette) under a new name and used for different purposes. The new palette can be saved locally and used with the given application, or globally and used for all HYDRUS applications. Users hence can in this way define different palettes for displaying water contents, pressure heads, concentrations, or temperatures. Since the Standard Palette can not be changed, once any color is changed, the program will request to save a new scale under a new name. The changed colors will be used for all displayed variables (not only the actual one).

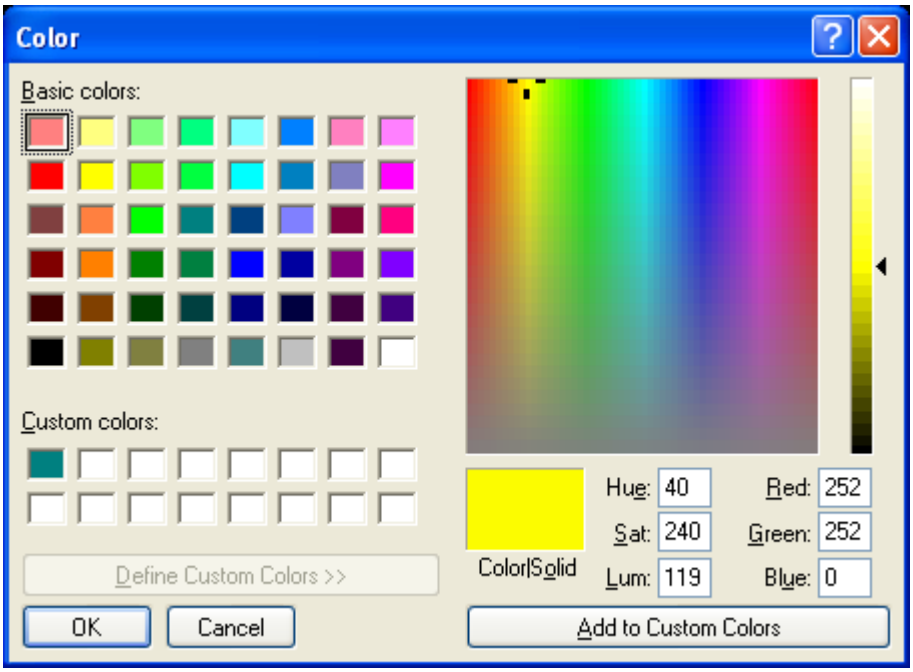


Figure 129. The Color dialog window.

Custom Scale

A user can define his/her own scale that is then remembered by the software and used for a particular variable in a given project. When one wants to use a certain scale also in other projects, he/she needs to save it using the **Save** command.

Other commands:

- **Default** – Sets the number of intervals to 11 and automatically fills values for the default scale

- **Empty** – Deletes all values (used with commands **Fill** and **Fill Max/Min**)
- **Fill** – Fills empty spaces between specified upper and lower values using linear interpolation
- **Fill Max-Min** – Similar to **Default**, except that this command does not set the number of values to 11 (it uses the number of values selected by a user)
- **Save** – Saves the Scale for use with other projects
- **Delete** – Deletes a selected **Custom Scale**

The number of values at the Scale can not be increased, it can only be lowered (from 11) using a "slider". By drawing a slider, one can also generate values at a Scale (see Figure 130):

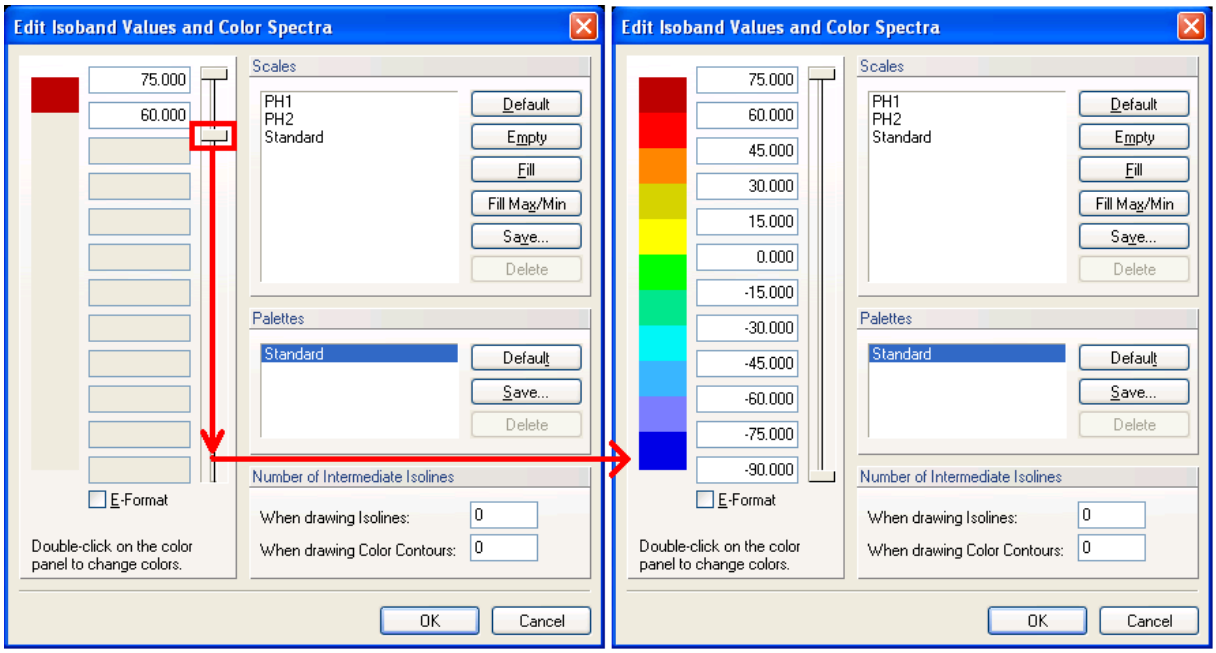


Figure 130. Adjusting scale in the Edit Isoband Value and Color Spectra dialog window.

When using a **Custom Scale**, the actual minimum or maximum of a displayed variable can be outside of the interval of the scale. Values outside of the interval of the scale are not displayed in the View window, resulting in empty spaces as shown in the upper part of see Figure 131.

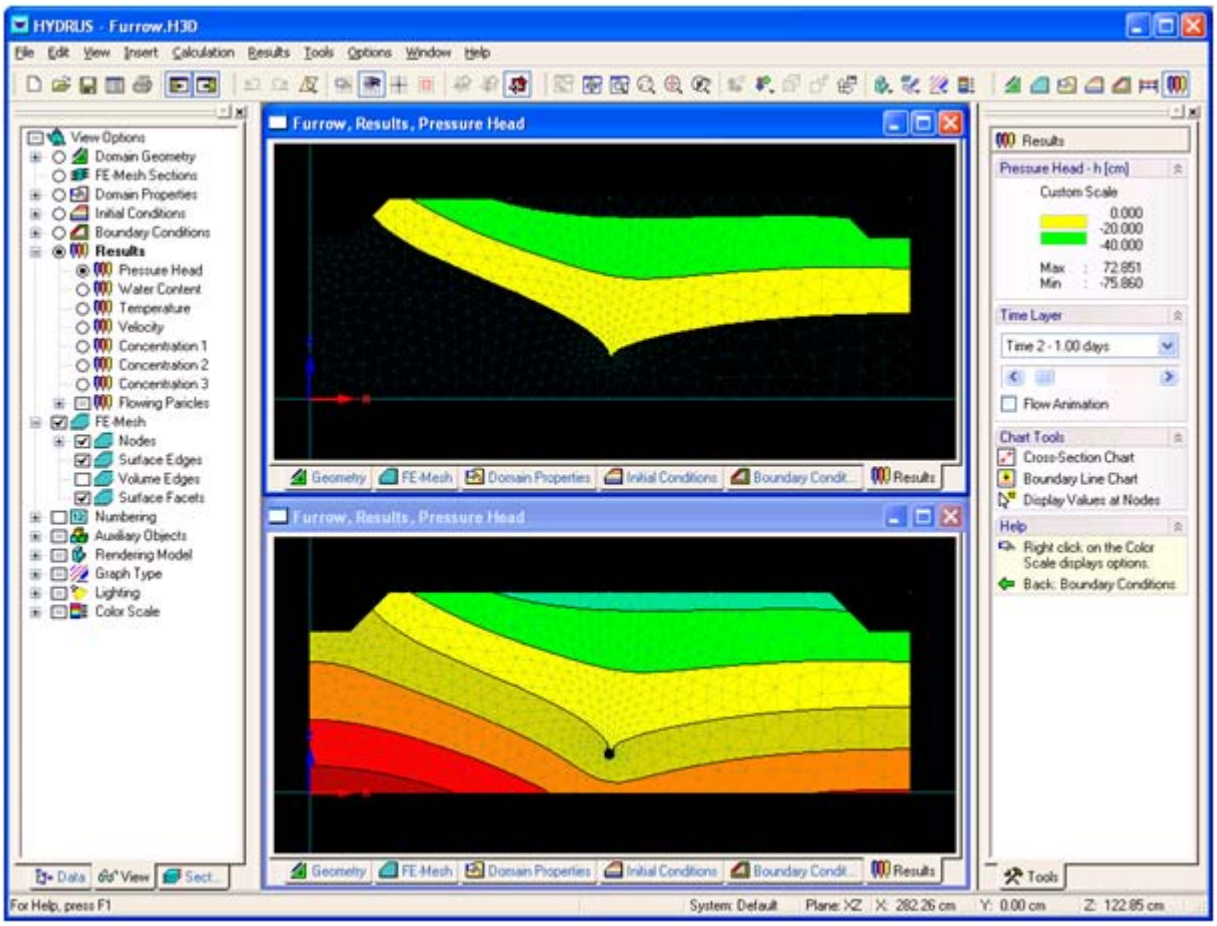


Figure 131. The use of the Custom Scale.

A **right** mouse button click on the Color Scale at the Edit Bar displays the menu for a fast change of various options related to scale.

- **Color Smoothing** – colors will change smoothly between particular iso-spectra corresponding to changes of the displayed variable (upper View at Figure 132).
- **Min/Max global in Time** - the scale of a certain variable is defined by the minimum and maximum of all values from all time levels
- **Min/Max global in Space** - the scale of a certain variable is defined by the minimum and maximum of all values over the entire transport domain
- **Standard Scale** – uses the Standard Scale, while the Custom Scale for a given variable (if it exists) is remembered
- **Custom Scale** – uses the Custom Scale if it exists. If it does not exist (default), this button is disabled. If one wants to use the Custom Scale, he/she needs to first create it in the **Edit Scale and Colors** dialog.
- **Edit Scale and Colors**

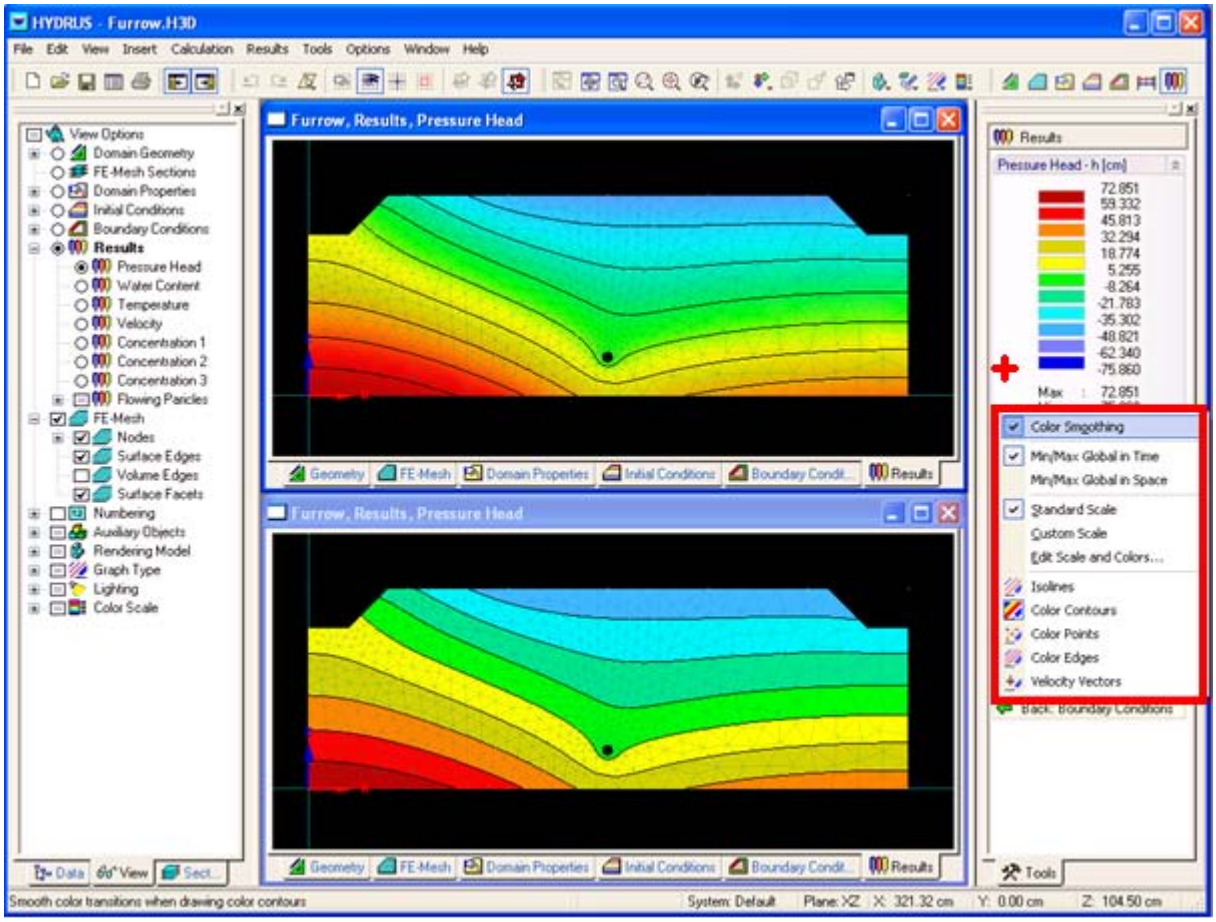


Figure 132. The color smoothing.

7.2. *Results – Other Information*

Additional information, such as boundary fluxes and/or soil hydraulic properties can be displayed using *x-y* graphs (**Results – Other Information** on the **Data Tab** of the **Navigator Bar**, or **Results Menu**, Fig. 133). Figure 133 shows the ***x-y* graph** dialog window that displays pressure heads in observation nodes.). Table 24 gives an overview of the different graph options that are possible. Two list boxes at the top of the ***x-y* graph** dialog window provide various combinations of graphs that are possible to display (Table 24). Browsing through various graphs is additionally also enabled using the *Previous* and *Next* command. Double-clicking at various objects of the ***x-y* graph** (e.g., axis, title, captions, legend) will allow users to redefine them, i.e., to change their text, colors, or fonts. When the right mouse button is clicked above the graph a pop-up menu will appear that will also allow users to redefine various objects of the ***x-y* graph**. One can for example change the text of both vertical and horizontal axis (*Axis->Title*) captions and titles (*Title*), their fonts, and colors, one can copy the content of the graph to the clipboard (*Copy*) for later paste in various other windows applications (e.g., MS Word, PowerPoint, or Excel), or one can change the thickness and colors of displayed lines. Many other modifications of the displayed ***x-y* graph** are possible. Data displayed in the ***x-y* graph** can be exported into an ASCII file using the *Export* command. The ***x-y* graph** settings can be saved using the *Save* command. Selected variable can be displayed either for all or for selected observation nodes.

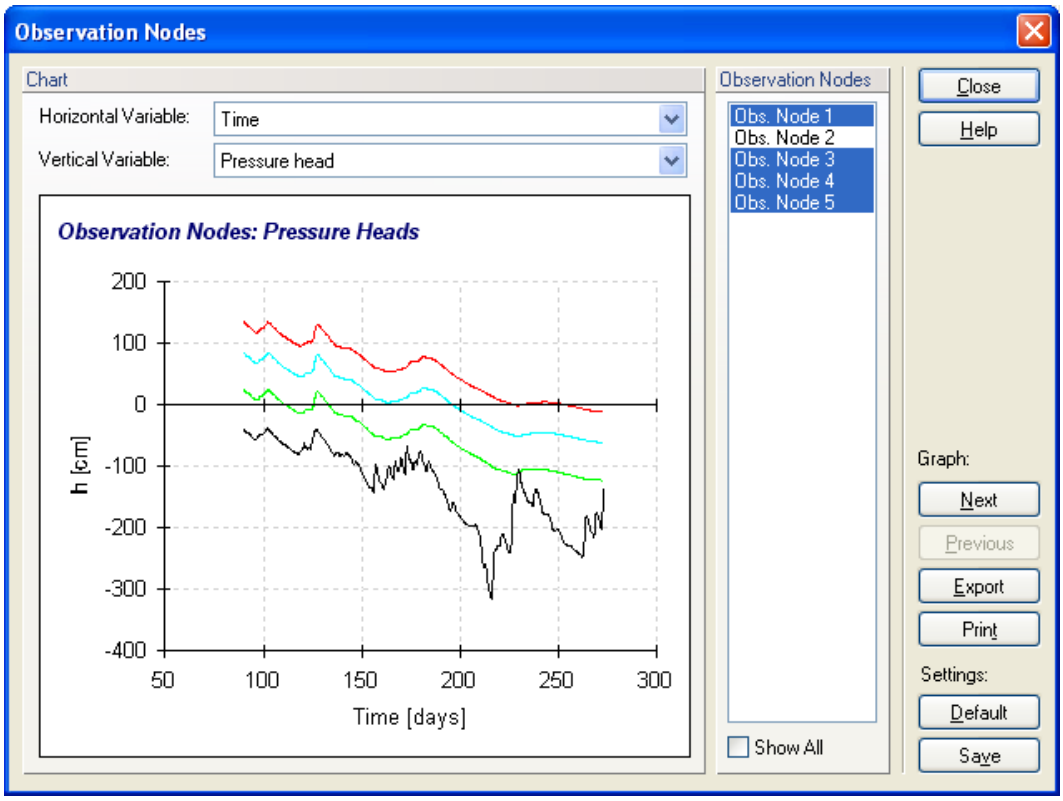


Figure 133. The *x-y* graph dialog window displaying pressure heads in observation nodes.

Table 24. Graph options in the HYDRUS interface.

Command	Horizontal Axis	Vertical Axis
Observation Points	Time	Pressure Head Water Content Temperature Concentration – x^+ Sorbed Concentration - x^+
Pressure Heads	Time	Atmospheric Boundary Head Root Zone Head Variable Boundary Head 1 Constant Boundary Head Seepage Face Head Drainage Boundary Head Free and Deep Drainage Boundary Head Variable Boundary Head 2 Variable Boundary Head 3 Variable Boundary Head 4 All Boundaries
Water Boundary Fluxes	Time	Potential Atmospheric Flux Potential Root Water Uptake Rate Actual Atmospheric Flux Actual Root Water Uptake Rate Variable Boundary Flux 1 Constant Boundary Flux Seepage Face Flux Drainage Boundary Flux Free and Deep Drainage Boundary Flux Variable Boundary Flux 2 Variable Boundary Flux 3 Variable Boundary Flux 4 All Atmospheric Fluxes All non-Atmospheric Fluxes
Cumulative Water Boundary Fluxes	Time	Potential Atmospheric Flux Potential Root Water Uptake Rate Actual Atmospheric Flux Actual Root Water Uptake Rate Variable Boundary Flux 1 Constant Boundary Flux Seepage Face Flux Drainage Boundary Flux Free and Deep Drainage Boundary Flux Variable Boundary Flux 2 Variable Boundary Flux 3 Variable Boundary Flux 4 All Boundaries Fluxes
Solute Fluxes$^+$	Time	Cumulative Zero-Order Reaction Cumulative First-Order Reaction Cumulative Root Solute Uptake Cumulative Non-Equil. Mass Transfer Cumulative Constant Boundary Solute Flux Cumulative Seepage Face Solute Flux

		Cumulative Variable Boundary 1 Solute Flux Cumulative Atmospheric Solute Flux Cumulative Drain Boundary Solute Flux Cum. Free/Deep Drainage Bound. Solute Flux Cumulative Variable Boundary 2 Solute Flux Cumulative Variable Boundary 3 Solute Flux Cumulative Variable Boundary 4 Solute Flux Constant Boundary Flux Seepage Face Flux Variable Boundary Flux 1 Actual Atmospheric Flux Drain Boundary Flux Free and Deep Drainage Boundary Flux Variable Boundary Flux 2 Variable Boundary Flux 3 Variable Boundary Flux 4 All Solute Cumulative Fluxes All Solute Fluxes
Soil Hydraulic Properties	Pressure Head Log Pressure Head Water Content	Water Content Soil Water Capacity Hydraulic Conductivity Log Hydraulic Conductivity Effective Water Content Pressure Head Log Pressure Head
Run-Time Information	Time Level Time	Time Step Number of Iterations Cumulative Number of Iterations Peclet Number Courant Number Number of Solute Iterations

[+] This graph is given for each solute

The *x-y graphs* have only a limited capacity and can display at most 6,000 data points and 20 lines. If a dataset to be displayed has more data points then allowed, then automatic selection is made by the program (only each *n* data point is displayed) and a warning (*File is too big to be displayed entirely! Automatic selection has been made.*) is issued. If the number of observation nodes is larger than 20, only the first 20 observation nodes are displayed.

Additional text output is provided under the command *Mass Balance Information* on the **Data Tab** of the **Navigator Bar** (also at the **Results Menu**). This output gives the total amount of water, heat and solute inside each specified subregion, and the inflow/outflow rates to/from that subregion, together with the mean pressure head (*hMean*), mean temperature (*TMean*) and the mean concentration (*cMean*) over each subregion (see Table 11.6 of the Technical Manual). Absolute and relative errors in the water and solute mass balances are also printed to this file. Output related to the inverse problem is provided under the command *Inverse Solution Results* on the **Data Tab** of the **Navigator Bar**. The *Chemical Mass Balance information* (on the **Data Tab** of the **Navigator Bar** or at the **Results Menu**) is provided for the Unsatchem module. This file gives mass balances

in different phases (liquid, sorbed, solid) for all major ions (i.e., Ca, Mg, Na, K, HCO3, SO4, and Cl).

The text dialog displaying *Mass Balance Information* or *Inverse Solution Results* had only a limited capacity in Version 1.x of HYDRUS. If the file to be displayed wass larger than this capacity (when there is too many print times or large number of data points in the inverse problem), a warning "*File is too big to be displayed entirely! Open it in any text editor.*" was given. Users in such case needed to display the *Balance.out* or *Fit.out* files, respectively, directly using any text editor, such as *Notepad* or *WordPad*. Both files are located in the *Temporary Working Directory* (see Section 1). This capacity problem was overcome in Version 2 and the dialog windows now displays the button *Next* (or *Previous*), which allows browsing through larger text files.

7.2.1. *Convert to ASCII*

The output files H.OUT, TH.OUT, CONCx.OUT, SORBx.OUT, TEMP.OUT, and V.OUT provide binary output of specific variables. The user interface can convert these binary files into the ASCII files H.TXT, TH.TXT, CONCx.TXT, SORBx.TXT, TEMP.TXT, and V.TXT using the **Convert to ASCII** dialog window (Fig. 134) (**Results – Other Information** on the **Data Tab** of the **Navigator Bar**, or *Results->Convert Output to ASCI*). The ASCII (text) files (e.g., h.txt, th.txt, v.txt) simply provide Print Time followed by a sequential list of values of a particular variable. These values are listed in the same order as Finite Element nodes. Coordinates for each FE node can be found in the MeshTria.txt file.

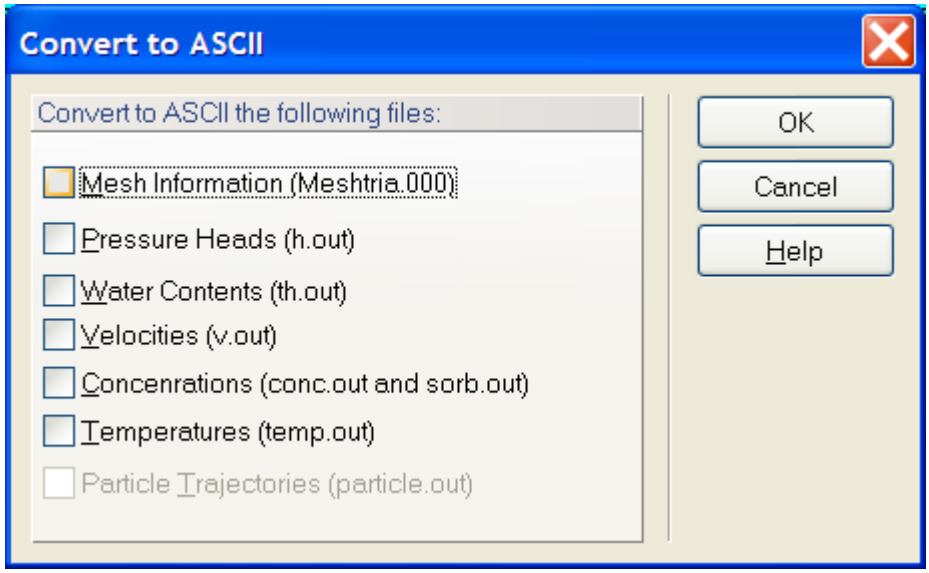


Figure 134. The Convert to ASCII dialog window.

8. Graphical User Interface Components

8.1. *View Window*

8.1.1. *Scene and Viewing Commands*

We will use here the term '**Scene**" for the content of the **View** window. Four types of commands are available to change the display of the **Scene** in the **View** window.

a) Commands to define a required **Display of the Scene**.
Detailed information about particular commands is given in Section 8.4. In addition to those commands, it is always possible to adjust the **Display of the Scene** using the "mouse scroll wheel" as follows:

- Simultaneously holding the mouse scroll wheel and moving the mouse will move the **Scene** in the same direction as the mouse, i.e., to the left, right, up, or down.
- Simultaneously holding the **Ctrl** keyboard button and the mouse scroll wheel, while moving the mouse, rotates the **Scene** around the center of the displayed object (available only for three-dimensional objects).
- Simultaneously holding the **Shift** keyboard button and the mouse scroll wheel, while moving the mouse, leads to zooming in or out of the **Scene** from the center of the **View** window.
- Rotating the scroll wheel (up or down) while pointing the mouse to a particular point in the View window results in zooming (in or out) the **Scene** from this point.
- Simultaneously holding the right mouse button and the mouse scroll wheel, while moving the mouse, rotates the **Scene** around the center of the displayed object (available only for three-dimensional projects).

The above described operations are available not only during selection (on existing transport domain), but also when defining basic geometrical objects. This allows users to adjust the View window as needed without interrupting the process of graphically defining objects of the transport domain.

b) Commands to define the **Content of the Scene**.
In every view one can independently specify what is to be displayed, e.g., a variable, the type of graph, or the numbering of objects. All possible options related to the **Content of the Scene** are located on the **Navigator Bar** of the **View Tab** (Section 8.2).

c) Displaying and/or hiding parts of complicated objects.
One often needs to display only some part of a complicated object while hiding the rest. For this purpose one can use commands related to **Sections** (i.e., parts of the computational domain or FE-Mesh). Detailed information is given in Chapter 8.1.8 on **Sections**.

d) Colors, fonts, and type of lines.

One can define colors, the style and thickness of lines, fonts for numbering, and other displaying options for almost all displayed/used objects. Separate default sets exist for the display for the screen and the printer. Users can create and save additional combinations of display options. Detailed information is provided in Chapter 7.1.1 on **Display Options**.

8.1.2. *Grid and Work Plane*

The **Grid and Work Plane** dialog window (Fig. 135) allows users to

a) select a **Work Plane** (i.e., a plane in which users can specify various boundary objects, initial and boundary conditions, or other information),
b) define the **Origin** of the coordinate system, and
c) define the *Alignment Grid*. The **Grid** is defined by its *Origin*, the type (*Grid Type*) of coordinate system involved (either *Cartesian* or *Polar*), and the *Grid Spacing*. The **Grid** can also be rotated to facilitate work, for example when defining the domain for a hill slope problem.

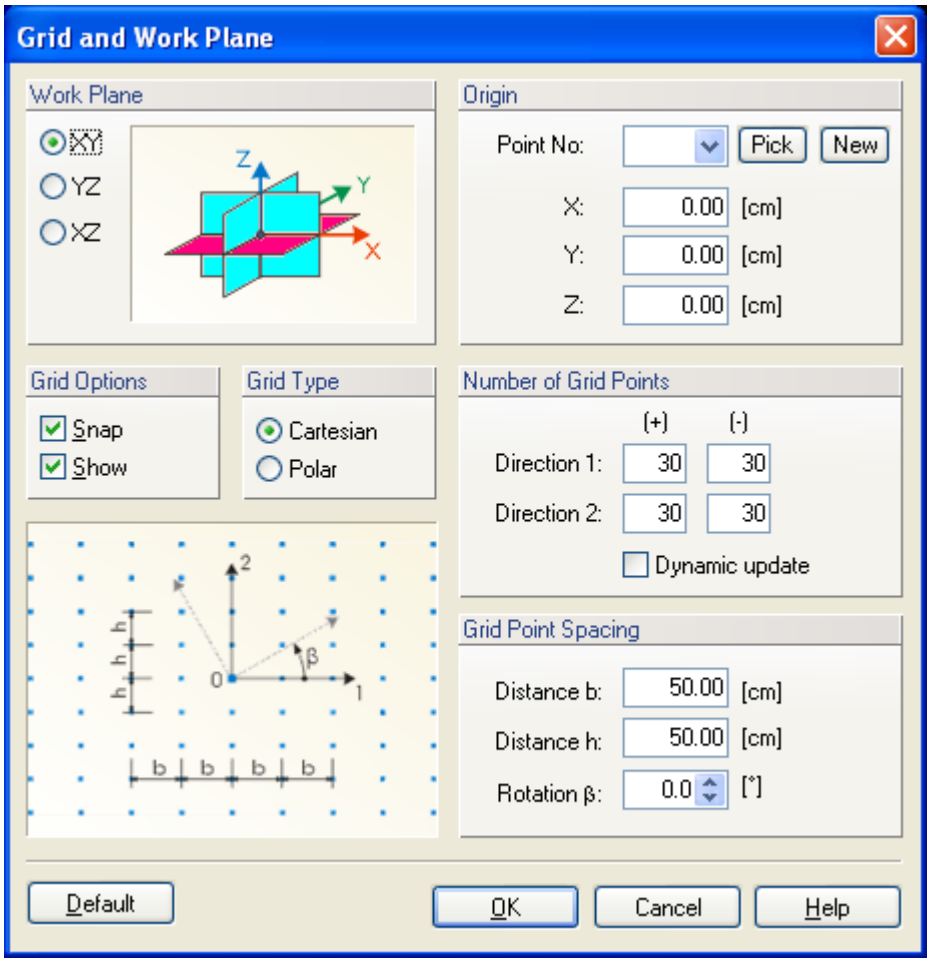


Figure 135. The Grid and Work Plane dialog window.

8.1.3. *Stretching Factors*

In many applications one direction of the transport domain dominates the other direction (or the other two directions). To facilitate work in the graphical environment, HYDRUS allows stretching of the domain in one (or two) direction(s) using **Stretching Factors**. This is done using the **View Stretching Factors** dialog window (Fig. 136) that is called with the command *View->View Stretching*.

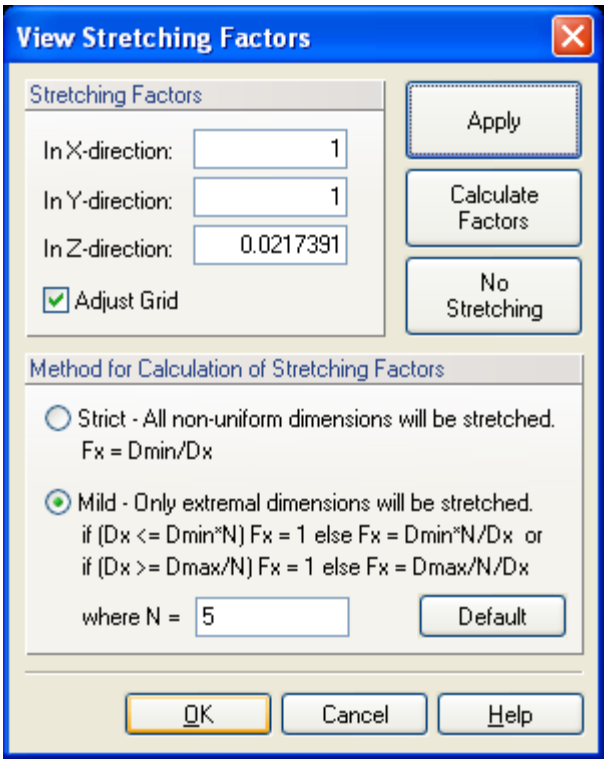


Figure 136. The View Stretching Factors dialog window.

Two options of View Stretching are available:

a) **Strict Stretching** when all transport domain dimensions will be displayed as being the same. For example a hexahedral of any dimensions will be displayed as a cube.

b) Mild Stretching, which adjust view stretching only when large differences in dimensions in different directions exist. By default there will be no view stretching when the larges dimension is 5 times larger than the smallest dimension.

A user should first select the **Method for Calculation of Stretching Factors** (either **Strict** or **Mild**), then click the command **Calculate Factors** (which will calculate stretching factors based on the method of stretching selected), and finally click the **Apply** command to update the **View Window**.

8.1.4. *Rendering Model*

Rendering serves to rapidly switching between displays of surfaces and solids. One can select the **Wire** and **Full Rendering** options. An advantage of **Wire Rendering** is mainly the speed of the display, while **Full Rendering** provides a more realistic display of three-dimensional objects.

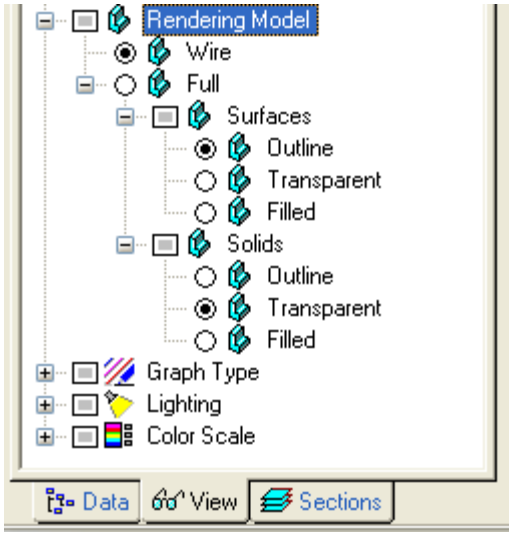


Figure 137. The Rendering part of the View Tab of the Navigator Bar.

8.1.5. *Selection and Edit Commands*

The **selection** of graphical objects is based on standards used in MS Office. An object is selected by clicking the left mouse button; a multiple selection is made by simultaneously holding the Shift button. A selection can be made using a rectangle (by clicking with the left mouse button outside of objects and holding the left mouse button while moving the mouse), rhomboid (see Chapter 8.4. on **Toolbars** and **Tools,** with the *Edit->Select->Select by Rhomboid* command), circle (*Edit->Select->Select by Circle*) or polygon (*Edit->Select->Select by Polygon*).

In the Standard Selection Mode (*Edit->Select->Standard Selection Mode*) the status of the selected object is changed (selected or unselected) after its selection, i.e., the selection is toggled. If we want to only add or remove objects to or from existing selection (i.e., we want to prevent switching the status of selected objects (toggling)), respectively, it is possible to choose two special selection modes: "Add to Selection" (*Edit->Select->Add to Selection*) or "Remove from Selection". (*Edit->Select-> Remove from Selection*). Both commands are accessible from the submenu *Edit->Select* or from the toolbar under the button "**Tools for Selection**". Two special Selection Modes can also be activated by holding the "Left Ctrl" (*Add to Selection*) or "Right Ctrl" (*Remove from Selection*) keyboard buttons.

When the cursor (mouse) is moved above an object, information about that object appears on the status bar and the object is temporarily highlighted; this process is referred to as **pre-selection**.

Apart from selecting objects graphically, they can also be selected using their **Indices** or by means of **Sections**.

Double-clicking on selected objects or simultaneous holding the Alt+Enter buttons recalls dialogs for editing properties of particular objects. Most dialogs support **multiple editing**, i.e., if edit boxes with different values remain empty, the original values will not change. This feature allows for example *Z*-coordinates of multiple selected points to be changed, while leaving the *X*- and *Y*-coordinates unchanged.

When different objects are selected simultaneously (e.g., points and curves), double clicking causes a dialog window to appear from which objects can be selected for editing.

8.1.6. *Pop-up Menus*

Context-sensitive menus with useful commands for a particular object can be called from the **View** window when clicking the right mouse button. While the commands are accessible also from the main menu, right-clicking the mouse is much faster. Menus for multiple selections that may contain different types of objects operate in the same way. When the right mouse button is clicked a default menu will appear when no object is close to the cursor.

When one clicks with the right mouse button on the view window, the pop-up menu of Figure 138 will appear. This menu will allow users to

a) select different views (*View*), i.e., Isometric, in *X*-direction, in *Y*-direction, in *Z*-direction, Reverse *X*-direction, Reverse *Y*-direction, Reverse *Z*-direction, or a perspective view.
b) select *Numbering* (turns on and off the display of numbering for objects selected under *Numbering Options* on the **Navigator Bar**).
c) go quickly to various *Numbering Options* (this command will bring the **Navigator Bar** to the View Tab on Numbering).
d) switch *Full Rendering/Wire Rendering* (see 8.1.4).
e) start the *Autorotate* function that will rotate the transport domain in the View window
f) call the *Show Work Plane*, i.e., to show the axis and the origin of the Work Plane
g) call the **Set Grid and Work Plane** dialog window (Fig. 135) (*Set Grid and Work Plane*)
h) select the *Coordinate System* (call the **List of Available Coordinate Systems** dialog window), and
i) call the **Display Options** dialog window (Fig. 126).

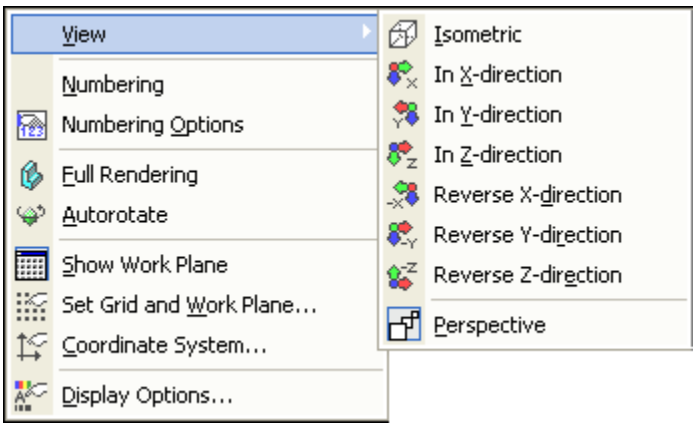


Figure 138. The Pop-up Menu from the View window.

8.1.7. *Drag and Drop*

By clicking and holding the left mouse button on selected objects in the **View** window, the **Drag and Drop** operation is started. This operation allows selected objects to be moved to a new location. Simultaneous holding the Ctrl keyboard button leads to the creation of a copy of the selected object. The copy can be moved into a different view, or in a different open project. The operation terminates by holding the Esc button or by clicking the right mouse button. **Drag and Drop** can be used for most geometric objects, but also for auxiliary objects such as comments, labels, and bitmaps.

Holding the Shift button during the **Drag and Drop** operation leads to movement of selected objects in a direction perpendicular to the current **Working Plane** (available only for three-dimensional objects).

8.1.8. *Sections*

Sections serve do divide complex objects (models) into simpler parts. Only the simpler parts are then displayed in the **View** window while the remaining parts are hidden. Two types of sections exists: those for geometric objects (**Geo Sections**) and those for the FE-Mesh (**FE-Mesh Sections**) (see also Section 5.7 and Table 19). New sections for both types can be created and named, a list of which is displayed on the **Section Tab** of the **Navigator Bar**. Clicking on the **Section** of the **Navigator Bar** causes the **Section** to be displayed in the **View** window. Multiple **Sections** can be displayed simultaneously by holding the “Shift” button during the selection. Undesired (to be displayed) parts can be cut off and hidden from the **View** window using the **Cut with Rectangle** command. This leads to a temporary section that is remembered by the program and renewed after the project is closed and reopened. New **sections** can be named and listed in the **Navigator Bar** by using commands to create new sections. The simplest menu command is the **New Section from the View** command (alternatively, one can use the **Create New Section from Current View** command from the Edit Menu of the Sections Tab of the Navigator Bar), which creates a newly named **section** from currently displayed objects in the **View** window. The **New Section from Selection** menu command (alternatively, one can use the **Create New**

Section from Selected Objects command from the Edit Menu of the Sections Tab of the Navigator Bar) creates a newly named section from currently selected objects or the FE-Mesh. The **Display Whole Domain** (**View All**) and **Display Whole FE-mesh** commands causes the entire computational domain or FE-Mesh to be displayed.

Geometrical Sections can be created manually (as described above) or automatically. The automatically generated **Geo Sections** are generated as follows. An object above each part of the **Base Surface** (in the 3D-Layered Domain) forms a **Column**, which is divided into **Layers**, depending on how many vertical layers the domain is divided into. Each such **Layer** of each such **Column** then forms one **Object** (a **Domain Section**). When we have *N* **Columns** (that is, *N* parts in the **Base Surface**) and the domain is divided into *M* horizontal **Layers**, then the number of generated objects is *N***M*. At the same time, **Surfaces** belonging to each of these objects are also generated. Some of these **Surfaces** are *Horizontal* and some are *Vertical* (although these terms are only approximate). **Surfaces** can then be used to specify **Boundary Conditions**.

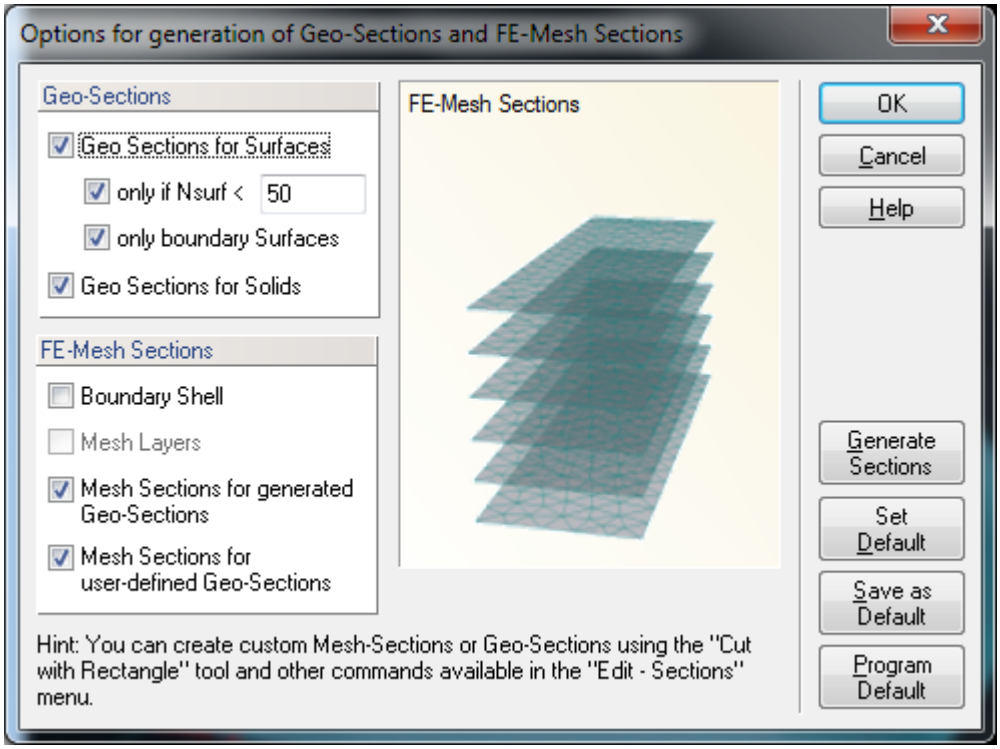

Options for generation of Geo-Sections and FE-Mesh Sections
Geo-Sections
Geo Sections for Surfaces
only if Nsurf < 50
only boundary Surfaces
Geo Sections for Solids
FE-Mesh Sections
Boundary Shell
Mesh Layers
Mesh Sections for generated Geo-Sections
Mesh Sections for user-defined Geo-Sections
FE-Mesh Sections
OK
Cancel
Help
Generate Sections
Set Default
Save as Default
Program Default
Hint: You can create custom Mesh-Sections or Geo-Sections using the "Cut with Rectangle" tool and other commands available in the "Edit - Sections" menu.

Figure 139. Options for Generation of Geo-Sections and FE-Mesh Sections dialog window.

Selected **Geo-Sections** and/or **FE-Mesh Sections** can be generated using the command **Generate Sections** in this dialog window (Fig. 139) obtained using the menu command *Edit->Sections->Generate Sections*. **Geo-Sections** can be generated either only for **Solids** or also for (Boundary and/or internal) **Surfaces**. Since working with **Geo-Sections** can be rather tedious when the number of **Surfaces** exceeds a certain limit, users can select this limit. The default setting (**Program Default**) is to generate **Geo-Sections** for up to 50 **Surfaces**. Note that the

number of **Surfaces** can be prohibitively large for certain **3D-Layered Domains** with multiple internal lines and/or layers. Users can therefore choose to generate FE-Mesh Section only for **Boundary Surfaces**, which are useful when specifying the boundary conditions, and not for internal Surfaces. User can change the default setting (**Program Default**), save it using the button **Save as Default**, and then recall it using the button **Set Default**. Note that different default setting can be saved for different types of domains.

Different **FE-Mesh Sections** are generated depending on the type of **Domain**. For the **3D-Layered Domains**, **FE-Mesh Sections** can be generated for the **Boundary Shell**, for each **Mesh Layer**, and for both automatically **Generated** and **User-Defined Geo-Sections**. For the **3D-General Domains**, **FE-Mesh Sections** can be generated for the **Boundary Shell**, and, again, for both automatically **Generated** and **User-Defined Geo-Sections**.

The **Partial View** is the status of the display (in the View window) when only part of the transport domain is displayed (i.e., only one or few, but not all, Sections are displayed). The parts that are not displayed are still visible in the background (gray thin lines and/or surfaces), but are inactive and cannot be selected for various operations. The **Partial View** can be cancelled (and the entire domain displayed) using the menu command **Cancel Partial View** or the popup menu command **Display Whole Domain**.

8.2. *Navigator Bars*

The **Navigator Bar** (Fig. 140) is by default located on the left side of the HYDRUS main window. A user can, however, move the **Navigator bar** to other positions. The **Navigator Bar** has three Tabs:

a) A **Data Tab** to allow quick access to all input and output data. Input data include *Domain Geometry*, *Flow Parameters*, *FE-Mesh*, *Domain Properties*, *Initial* and *Boundary Conditions*, and *Auxiliary Objects*. Output data include various *Results*. Data are organized in a tree-like structure. Figure 140 shows *Data* with expanded *Domain Properties* on the left and *Results* in the middle.
b) A **View Tab** (on the right of Figure 140) to specify what and how information will be displayed in the *View window*, and
c) A **Sections Tab** to show various Sections (not shown here and defined elsewhere).

View Options on the **View Tab** of the **Navigator Bar** at first mirror more or less the **Project Data**, i.e., **View Options** exists for *Domain Geometry*, *FE-Mesh*, *Domain Properties*, *Initial* and *Boundary Conditions*, and *Results*. Users can then select which objects (*Domain Geometry objects*, *Domain Properties objects*, *FE-Mesh objects*, *such as nodes*, *edges*, *triangles*, and *tetrahedrals*) are to be numbered (*Numbering*), display *Auxiliary Objects*, and initiate *Rendering* (*Outline*, *transparent*, *filled*). Users can also select the *Graph Type* (*Isolines*, *Isosurfaces*, *Contours* with or without *Separation Lines*, and *Color Edges*, *Color Points*, and *Velocity Vectors*) and *Color Scale* (either with or without *Min/Max glob. in time* or *Min/Max glob. in space*). Finally, *Lighting* can be turned on or off; the location of light sources can be shown (*Show Light Sources*), and the location of lights can be selected (*Light Switches*).

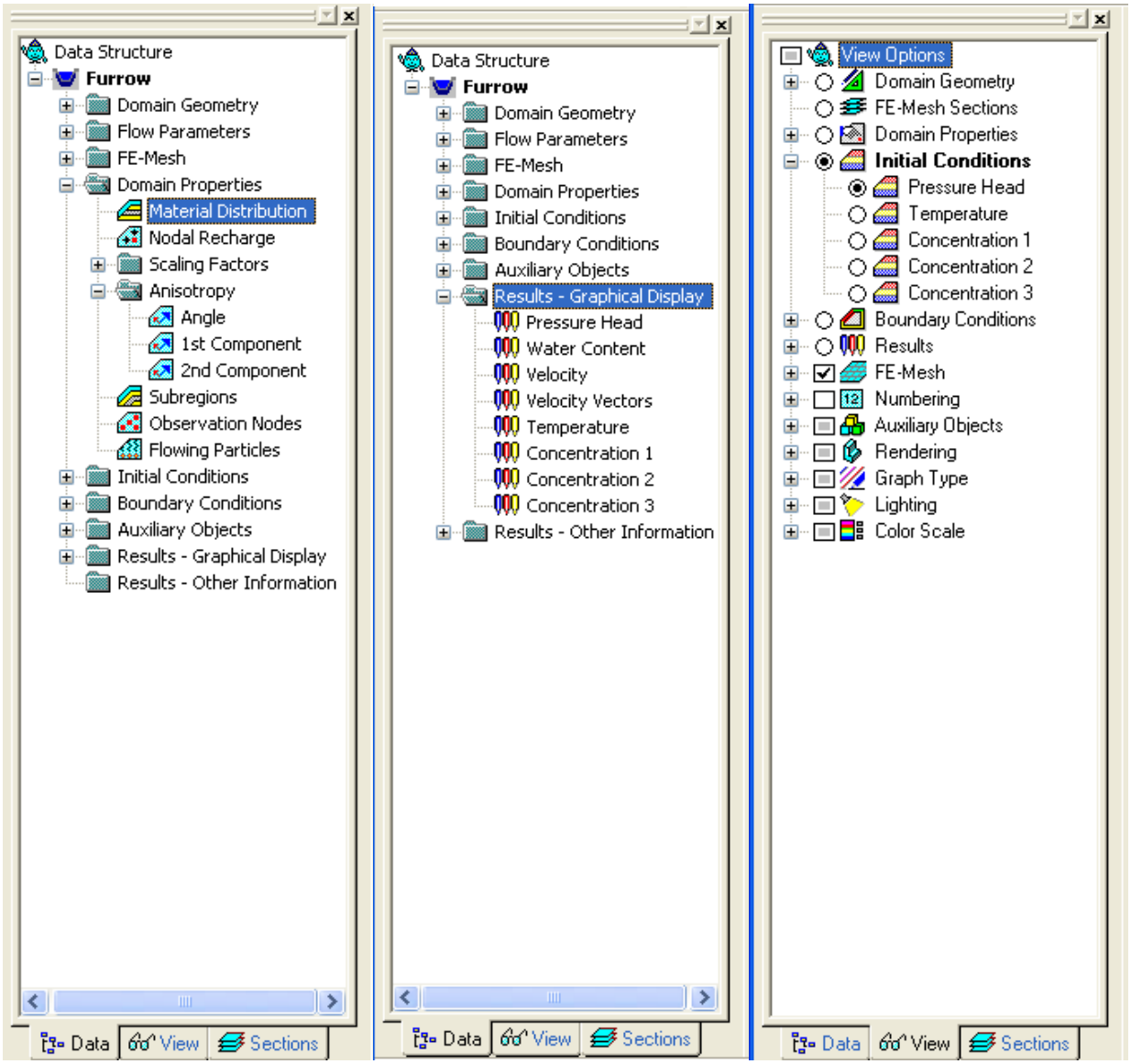


Figure 140. Selected Navigator Bars (Data Tabs on the left and in the middle, the View Tab on the right).

8.3. *Edit Bars*

The **Edit Bar** is by default located on the right side of the HYDRUS main window. A user can, however, move the **Edit Bar** to other positions. The **Edit Bar** is very dynamic since it changes depending upon the process being carried out. Figure 141 shows the **Edit Bars** for different processes, i.e., for the Material Distribution in the *Domain Properties*, the Water Flow *Boundary Conditions*, the Pressure Head *Initial Conditions*, and the Water Content *Results*.

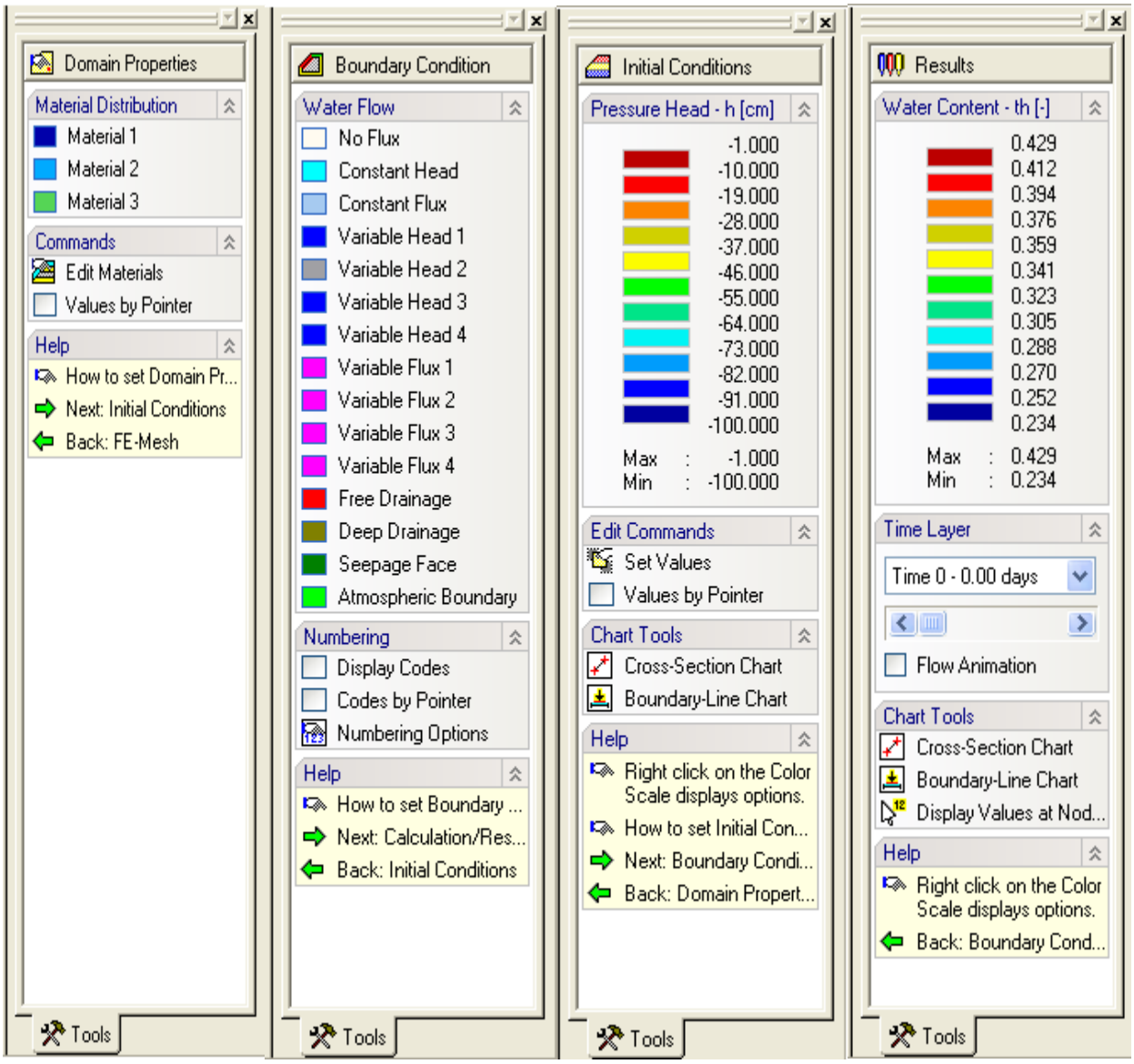


Figure 141. Selected Edit Bars (from left to right) for Material Distribution in Domain Properties, Water Flow Boundary Conditions, Pressure Head Initial Conditions, and Water Content Results.

As an example, the **Edit Bar** for **Domain Properties** and **Material Distribution** displays materials that can be assigned to selected nodes (in this case Materials 1, 2, and 3), the Command **Edit Materials** (which calls the **Water Flow Parameters** dialog window, Fig. 19), the command **Values by Pointer** (which displays the material number for a node closest to the cursor), and **Help**. The **Help** part of the **Edit Bar** usually contains help on a particular process (*How to* …), and the direction of the data inputting process (next or backwards).

The **Edit Bar** for **Boundary Conditions** and **Water Flow** displays the various boundary conditions that can be specified along boundaries of the transport domain, as well the command **Display Codes** (which displays boundary codes for all boundary nodes in the View window), the command **Codes by Pointer** (which displays boundary codes only for the node closest to the cursor), **Numbering Options** (which changes the **Navigator Bar** to the **View** Tab and *Numbering* option), **Boundary Conditions Options** (which allows additional system-dependent boundary conditions for water flow, see the Technical manual and Fig. 110), and **Help** (which is similar as discussed above).

The **Edit Bar** for **Initial Conditions** and **Pressure Head - h** displays a color spectrum that is used to draw the initial conditions, and lists the minimum and maximum values that are used in the entire domain. This **Edit Bar** also includes:

a) **Edit Commands**: **Set Values** and **Values by Pointer**. When nodes for which the initial conditions are to be specified are already selected, then the **Set Values** command calls the **Water Flow Initial Condition** dialog window (Fig. 107). When no nodes are selected, then clicking on the **Set Values** command causes a square cursor to appear, which may be used to select particular nodes, after which the **Water Flow Initial Condition** dialog window appears. The command **Values by Pointer** again displays the initial pressure head of the node closest to the cursor.
b) Two **Chart Tools** commands: The **Cross-Section Chart** and the **Boundary-Line Chart**. The **Cross-Section Chart** command allows users to display a particular variable between any two points of the transport domain. The **Boundary-Line Chart** command allows users to display a particular variable between any two points on the boundary of the transport domain, or along any line that is drawn along edges of finite elements within the transport domain. This line hence does not have to be straight, but can turn in any direction along finite element edges.
c) The **Help** commands as before.

The **Edit Bar** for **Results** and **Water Content** displays, similarly as for the initial conditions, a spectrum that is used to draw results, and the minimum and maximum values for the entire domain. This bar further includes:

a) A **Time Layer** command to specify which time layers (corresponding to print times specified in the **Output Information** dialog window, Fig. 16) are to be displayed. Time layers can be chosen either from the list box, or from a scroll bar. It is also possible to perform animation of results by clicking on the **Flow Animation** check box.
b) Two **Chart Tools** commands (**Cross-Section Chart** and **Boundary-Line Chart**), which have the same purpose as above for the initial condition. The last command (i.e., **Display Values at Nodes**) again causes the value of a particular variable (e.g., water content) of the node closest to the cursor do be displayed.

c) The **Help** command. One useful feature of the **Help** command here is the *Right click on the Color Scale displays options* (a right-click displays the **Edit Isoband Value and Color Spectra** dialog window, Fig. 127). Right-clicking results in the display of the pop-up menu (Fig. 142) that allows users to choose different display options, such as *Color Smoothing*, *Isolines*, and *Isobands*. These options are defined in more detail below.

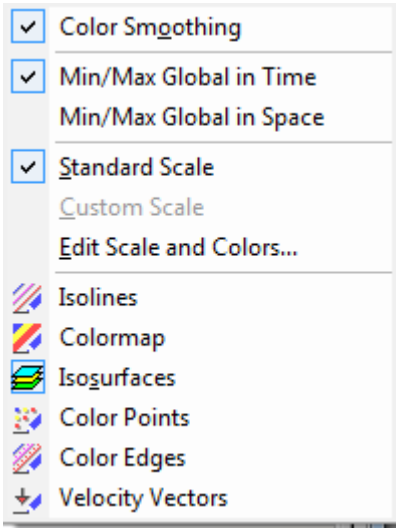


Figure 142. The Color Scale Display Options menu.

Color Smoothing	Colors are by default constant between isolines, but change abruptly at the isoline. Colors change gradually when this option is checked.
Min/Max Global in Time	The minimum and maximum values for the color spectrum are selected based on minimum and maximum values of a certain variable during the entire simulation.
Min/Max Global in Space	The minimum and maximum values for the color spectrum are selected based on minimum and maximum values of a certain variable in the entire transport domain (even when only part of the domain is displayed, e.g., one horizontal layer).
Standard Scale	Users can select between a standard or user-defined scale.
Custom Scale	Users can select between a standard or user-defined scale.
Edit Scale and Colors	Calls the **Edit Isoband Value and Color Spectra** dialog window (Fig. 127).
Isolines	Displays a selected variable using isolines.
Colormap	Displays a selected variable using isobands (color spectrum).
Isosurfaces	Displays a selected variable using isosurfaces.
Color Points	Displays a selected variable using color points.
Color Edges	Displays a selected variable using color edges.
Velocity Vectors	Displays velocities using velocity vectors.

Figure 143 shows two more **Edit Bars**, i.e., those for *Domain Geometry* and *FE-Mesh*. The **Insert Object** of the **Domain Geometry Edit Bar** allows users to **Insert Objects** with which a

transport domain is defined (i.e., points, lines, arcs, circles, splines, surfaces), as well as auxiliary objects such as dimensions and comments. The **Edit Objects** part allows objects to be edited using various actions, such as *Move*, *Copy*, *Rotate*, and *Mirror*. This **Edit Bar** also provides **Help** on how to *Edit Domain Geometry*, and to *Check Domain Definition.*

The **FE-Mesh Edit Bar** allows quick access to various commands needed for editing and generating the finite element mesh (**Edit FE-Mesh**), such as the *FE-Mesh Generator* (Fig. **Error! Bookmark not defined.**), *FE-Mesh Parameters* (Figs. 92 through 95), *Insert Mesh Refinement* (Fig. 97), *Delete All Refinements*, *Generate FE-Mesh*, *Delete FE-Mesh*, and *FE-Mesh Information* (Fig. 104). The **FE-Mesh Edit Bar** also allows users to generate the finite element mesh step by step (**FE-Mesh Advanced**), i.e., using individual steps such as *Fundamental Triangulation*, *Mesh Refinement*, *Delaunay Retriangulation*, *Convex Retriangulation*, and *Mesh Smoothing*. This **Edit Bar** additionally provides tools to work with **FE-Mesh Sections**, allows users to select how to make selections (**FE-Mesh Sections**) and **Help**.

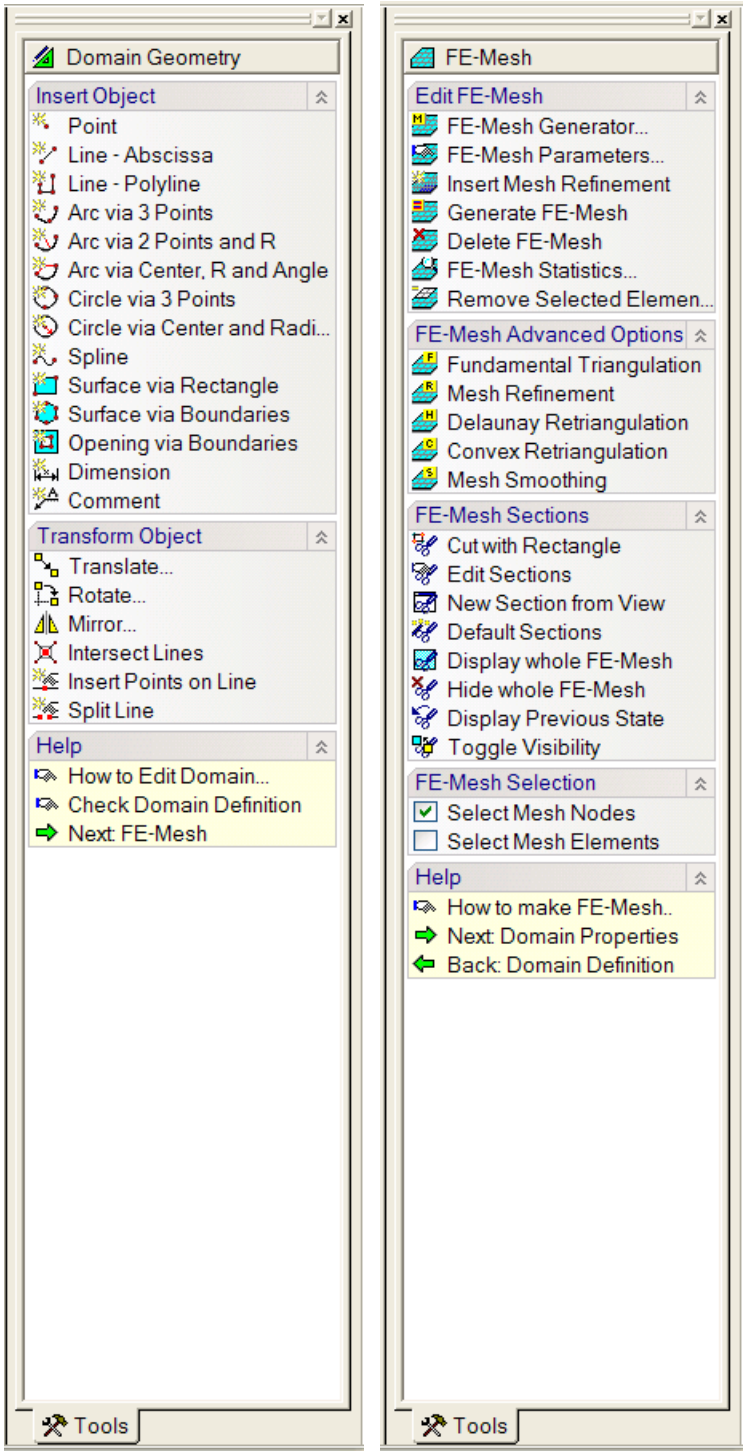


Figure 143. Selected Edit Bars (for Domain Geometry and FE-Mesh).

8.4. *Toolbars*

Users can use various **toolbars** that allow an easy access to the most frequently used commands. These commands are grouped into five toolbars that can be displayed using the command *View->Toolbars* (Fig. 144). Users can also create their own toolbars and customize them in various ways using the **Customize** dialog window (Fig. 145).

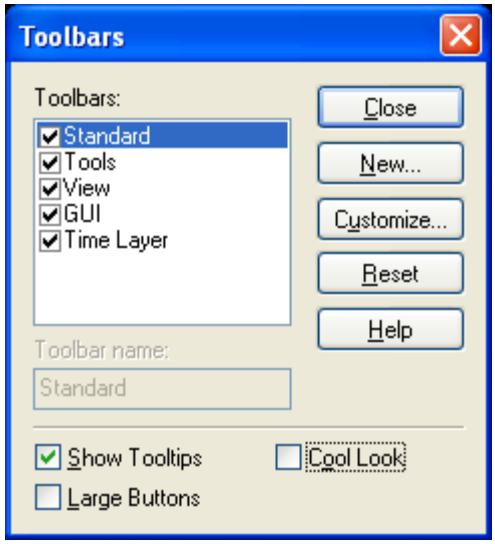


Figure 144. The Toolbars dialog window.

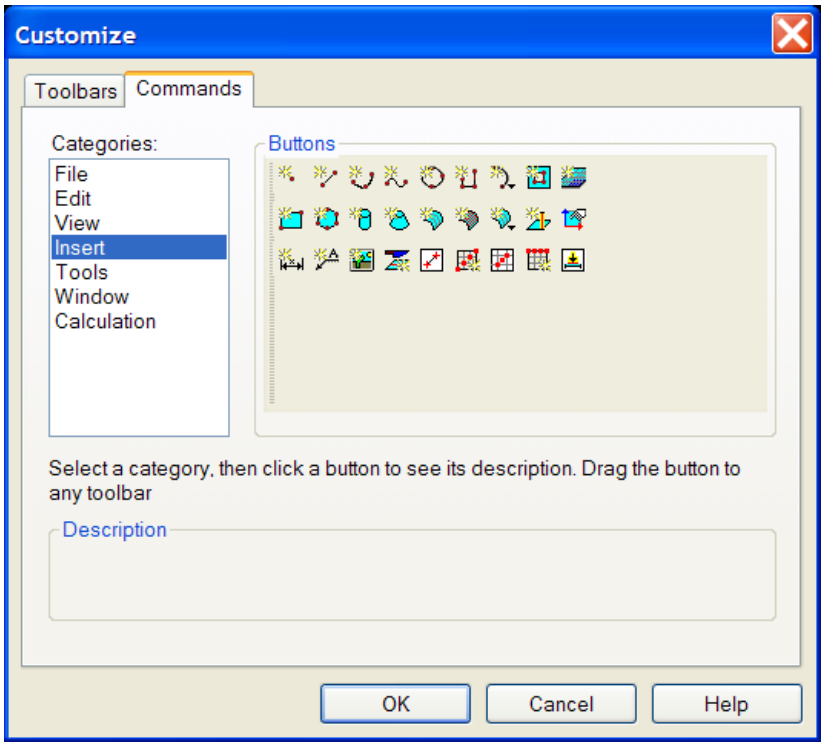
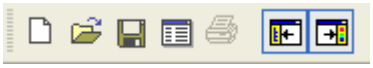


Figure 145. The Customize Toolbars dialog window.

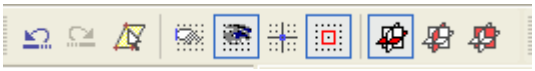
The default toolbars (i.e., **Standard Toolbar**, **Tools Toolbar**, **View Toolbar**, **GUI Toolbar**, and **Time Layer Toolbar**) are briefly summarized below (definitions in each case are from left to right).

a) Standard Toolbar:



New Project	Creates a new project.
Open a Project	Opens an existing project (represented by the *project_name*.h3d2 file)
Save Project	Saves the input data of the current project specified in the main program module if the data were either newly created or changed during an application run.
Project Data Manager	Calls the project manager to manage data of existing projects; helps to locate, open, copy, delete or rename the desired projects and their data (Figs. 2 and 3).
Print (Ctrl+P)	Prints the content of the View window.
Navigator Window	Displays or hides the Navigator Window.
Edit Bar	Displays or hides the Edit Bar.

b) Tools Toolbar:



Undo	Reverses the last edit actions.	
Redo	Repeats the last edit actions.	
Tools for Selection	Select by Rhomboid	Selects objects using rhomboid.
	Select by Circle	Selects objects using circle.
	Select by Polygon	Selects objects using polygon.
	Add to Selection	Add additional objects to existing selection.
	Remove from Selection	Remove objects from existing selection.
	Standard Selection Mode	
Grid and Work Plane Settings	Calls the Grid and Work Plane dialog window (Fig 135).	
Show Grid	Shows a Work Plane (axis and origin of the grid) in the View window.	
Set Grid Origin	Redefines the origin of the grid.	
Snap to Grid	Mouse moves in steps given by the grid.	
Set XY-Work Plane	Sets Work Plane to the XY plane.	
Set YZ-Work Plane	Sets Work Plane to the YZ plane.	
Set XZ-Work Plane	Sets Work Plane to the XZ plane.	

c) View Toolbar:

Rotate View	Allows objects in the View windows to be rotated using the mouse while holding the left mouse button.
Scroll View	Allows moving (scrolling) of objects in the View window using the mouse while holding the left mouse button.
Zoom View	Allows zooming of objects in the View window using the mouse while holding the left mouse button.

Similar functions can be achieved by pressing various buttons on the keyboard. **Rotating** is achieved by holding simultaneously the **Ctrl** button on the keyboard and the left mouse button. **Scrolling** occurs by holding simultaneously the **Shift** button on the keyboard and the left mouse button. And finally, **zooming** is achieved by holding simultaneously the **Alt** button on the keyboard and the left mouse button.

Zoom by Rectangle	Zooms in on a certain part of the View window using a rectangle.
View All	Shows the default view of the View window.
Previous view	Shows the previous view of a certain part of the View window.
In Reverse Z-direction	Sets the view of the transport domain in the reverse *Z*-direction.
View Commands	Shows a pop-up menu with the following commands: *Isometric* *In X-direction* *In Y-direction* *In Z-direction* *In Reverse X-direction* *In Reverse Y-direction* *In Reverse Z-direction* *Perspective* *Default View*
Isometric View	Specifies the isometric view.
Perspective View	Specifies the perspective view.
View Stretching Factors	Calls the View Stretching Factors dialog window (Fig 136).
Rendering Commands	Displays a menu with three commands on how to display the transport domain (see 8.1.4):
Full Model	Displays the transport domain as a full object.
Transparent Model	Displays the transport domain as a transparent object.
Wire Model	Displays the transport domain as a wired object.
Sections Commands	Displays a menu with nine commands for editing sections:

Cut with Rectangle
Cut with Indexes
Create New Section from Selection
Create New Section from Current View
Display All
Display Previous
Hide Selection
Display only Selection
Display Reverse
Edit Section

Graph Type Commands	Displays a menu with five commands.

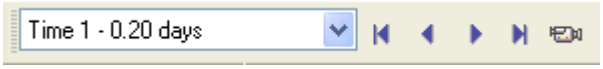
Isolines	Displays the spatial distribution of a certain variable by means of isolines.
Colormap	Displays the spatial distribution of a certain variable by means of color contours.
Isosurfaces	Displays the spatial distribution of a certain variable by means of isosurfaces.
Color Points	Displays the spatial distribution of a certain variable by means of color points.
Color Edges	Displays the spatial distribution of a certain variable by means of color edges.
Velocity Vectors	Displays Darcy velocity vectors.
Color Scale Options	Displays menu with seven commands:

Color Smoothing
Surface Lighting
Min/Max Values Global in Time
Min/Max Values Global in Space
Standard Scale
Custom Scale
Edit Scale and Colors

d) GUI Toolbar:

View/Edit Domain Geometry	Sets the View window to View/Edit Domain Geometry mode.
View/Edit FE-Mesh	Sets the View window to View/Edit FE-Mesh mode.
View/Edit Domain Properties	Sets the View window to View/Edit Domain Properties mode, to edit materials.
View/Edit Initial Conditions	Sets the View window to View/Edit Initial Conditions mode, to edit pressure head initial conditions.
View/Edit Boundary Conditions	Sets the View window to View/Edit Boundary Conditions mode, to edit water flow boundary conditions.
Execute Calculation	Executes a HYDRUS version 3.0 FORTRAN application.
View Results	Sets the View window to View Results mode, to view the pressure head distribution.

e) Time Layer Toolbar:



List box of Time Layers	Displays a list box with Time Layers with available results.
First Time Layer	Displays the first time layer.
Previous Time Layer	Displays the previous time layer.
Next Time Layer	Displays the next time layer.
Last Time Layer	Displays the last time layer.
Flow Animation	Displays time layers of a particular variable consecutively and continuously.

8.5. *HYDRUS Menus*

The main window of HYDRUS contains a menu that has ten submenus, i.e., File, Edit, View (Fig. 146), Insert, Calculations, Results (Fig. 147), Tools, Options, Windows, and Help (Fig. 148). Table 25 lists the main groups, the main menu items, as well as the main submenu and sub-submenu commands. Table 26 then provides brief descriptions of all menu commands.

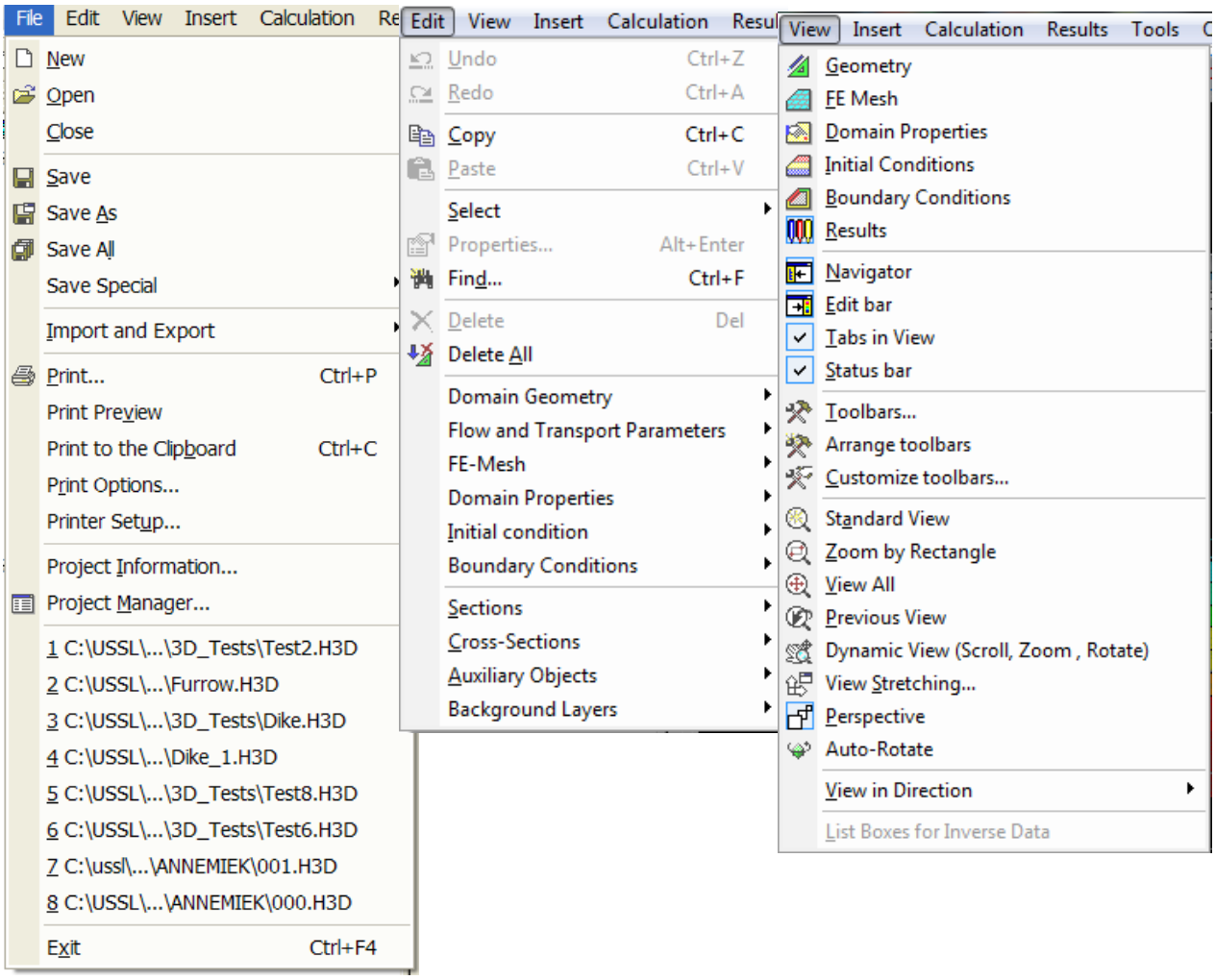


Figure 146. The HYDRUS Menus I (File, Edit, and View).

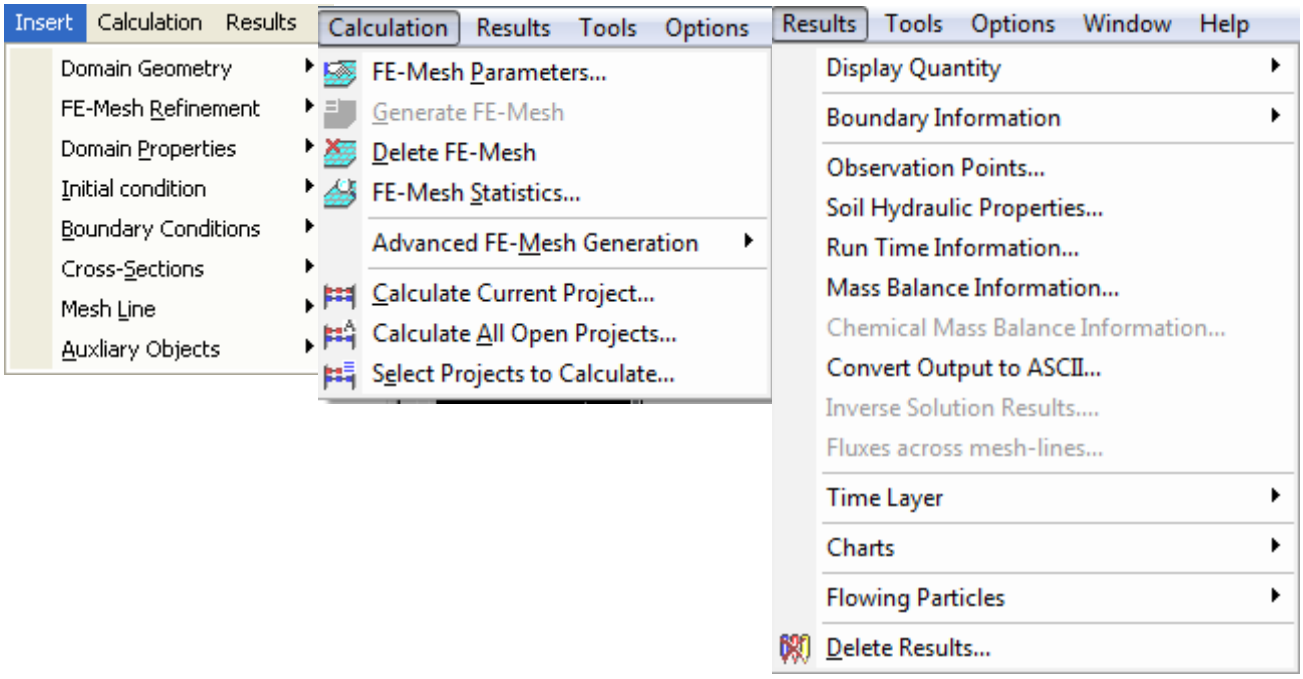


Figure 147. The HYDRUS Menus II (Insert, Calculations, and Results).

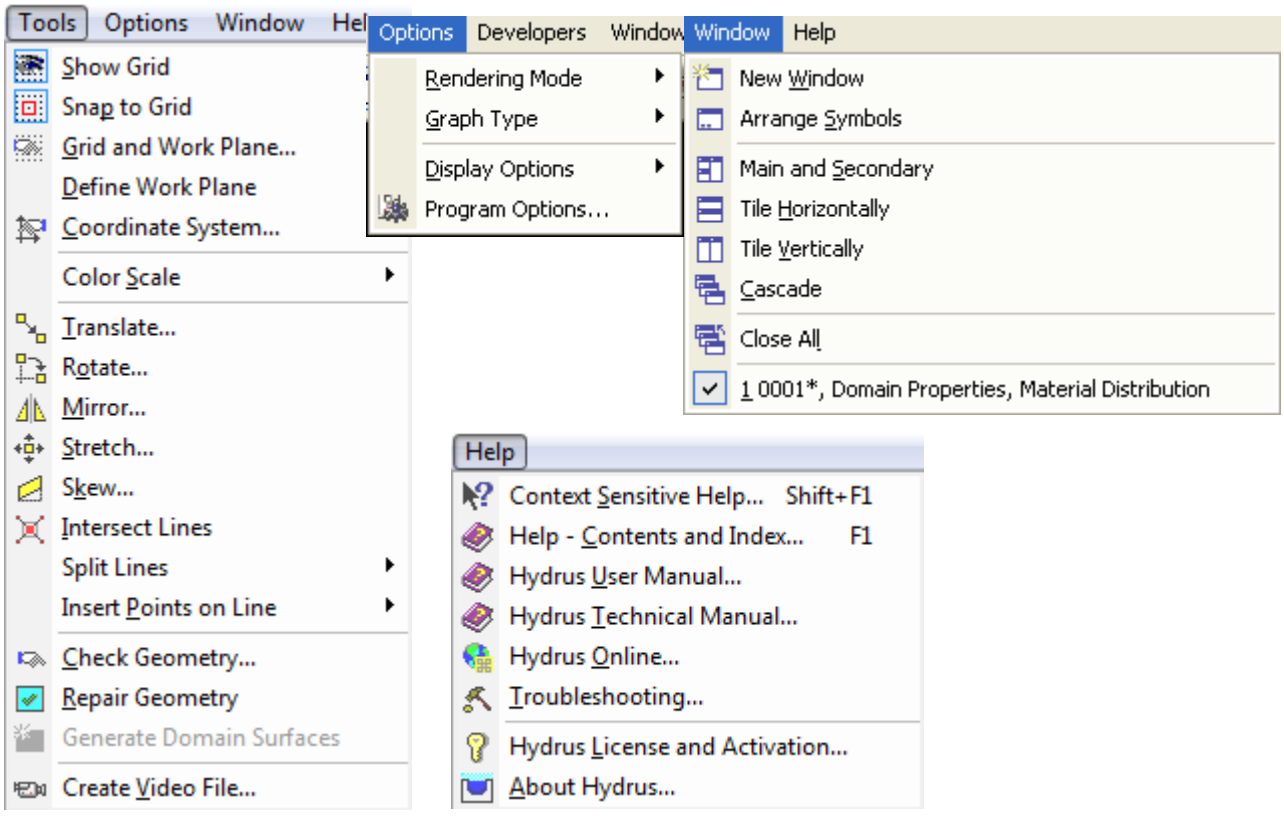


Figure 148. The HYDRUS Menus III (Tools, Options, Windows, and Help).

Table 25. HYDRUS menu commands.

Group	Menu	Submenu	Sub-Submenu
A File	New		
	Open		
	Close		
	Save		
	Save As		
	Save All		
	Import and Export	Import Hydrus-2D Project	
		Import Input Data from *.IN Files	
		Import Input Data from another HYDRUS Project	
		Export Data for Hydrus Solver in Text Format	
		Export Data to ParSWMS	
		Read Points from a Text File	
		Import Geometry from a Text File	
		Import Geometry from a DXF File	
		Import Geometry from a TIN File	
		Export Geometry to a Text File	
		Export only Selected Objects	
		Import Data from ParSWMS	
	Print		
	Print Preview		
	Print to the Clipboard		
	Print Options		
	Print Setup		
	Project Information		
	Project Manager		
	Recent Files		
	Exit		
B Edit	Undo		
	Redo		
	Copy		
	Paste		
	Select	Select by Rhomboid	
		Select by Circle	
		Select by Polygon	
		Add to Selection	
		Remove from Selection	
		Standard Selection Mode	
	Properties		
	Find		
	Delete		
	Delete All		
	Domain Geometry	Domain Type and Units	
		Simple Domain	
		3D-Layered Domain	
		Delete 3D-Layered Domain	

	Points	
	Lines	
	Surfaces	
	Openings	
	Thickness Vectors	
	Solids	
Flow Parameters	Main Processes	
	Inverse Solution	
	Time Information	
	Output Information	
	Water Flow Parameters	Iteration Criteria
		Hydraulic Properties Model
		Soil Hydraulic Parameters
		Anisotropy Tensors
	Solute Transport Parameters	General Information
		Solute Transport Parameters
		Solution Composition
		Solute Reaction Parameters
		Wetlands Parameters I
		Wetlands Parameters II
		Temperature Dependence
		Water Content Dependence
		Chemical Parameters
		Fumigant Application
	Heat Transport Parameters	
	Root Water Uptake	Root Water Uptake Models
		Pressure Head Reduction
		Osmotic Head Reduction
	Variable Boundary Condition	
	Data for Inverse Solution	
FE-Mesh	FE-Mesh Parameters	
	Generate FE-Mesh	
	Delete FE-Mesh	
	Remove Selected FE-Elements	
	FE-Mesh Statistics	
	Advanced FE-Mesh Generation	Fundamental Triangulation
		Mesh Refinement
		Homogeneous Triangulation
		Check of Convexity
		Mesh Smoothing
	Select Mesh Nodes	
	Select Mesh Elements	
Domain Properties	Material Distribution	
	Root Distribution	
	Nodal Recharge	
	Scaling Factor	Hydraulic Conductivity
		Pressure Head
		Water Content
	Local Anisotropy	Angle
		First Component
		Second Component
		Index
	Subregions	
	Observation Nodes	Edit in View
		Delete

		Clear All
	Drains	Edit in View
		Delete
		Clear All
		Drain Parameters
	Flowing Particles	Edit in View
		Delete
		Clear All
	Stochastic Distribution of S.F.	
	Subregions = Material Distribution	
	Nonequilibrium Conc. = a * Equil. Conc.	
	Parameters for Root Distribution	
	Delete All Domain Properties	
	Default Domain Parameters	
Initial Conditions	Pressure Head/Water Content	
	Concentration	
	Nonequilibrium Concentration	
	Temperature	
	Import	
	Delete All Initial Conditions	
Boundary Conditions	Water Flow	
	Solute Transport	
	Heat Transport	
	Boundary Conditions Options	
	Delete All Boundary Conditions	
Properties and Conditions on FE-Mesh		
Model Sections	Edit Sections	
	Generate Sections	
	New Section from Selection	
	New Section from View	
	Display Whole Domain	
	Display Previous	
	Hide Selection	
	Display only Selection	
	Display Reverse	
	Cut with Rectangle	
	Cut with Indexes	
	Import FE-Mesh Sections	
Cross-Sections	Edit	
	Delete Selected	
	Delete All	
	Auto-Adjust Work Plane	
Auxiliary Objects	Dimensions	Delete Selected
		Delete All
	Comments	Edit
		Delete Selected
		Delete All
Background Layers	Edit	
	Move	
	Rotate	
	Mirror	
	Stretch	
	Skew	

			Delete All
C View	Geometry FE Mesh Domain Properties Initial Conditions Boundary Conditions Results		
	Navigator Edit Bar Tabs in View Status Bar		
	Toolbars Arrange Toolbars Customize Toolbars		
	Standard View Zoom by Rectangle View All Previous View Dynamic View (Scroll, Zoom, Rotate) View Stretching Perspective Auto-Rotate		
	Cancel Partial View		
	View in Direction	Isometric In X-direction In Y-direction In Z-direction Reverse X-direction Reverse Y-direction Reverse Z-direction	
	List Boxes for Inverse Data		
D Insert	Domain Geometry	Points	Graphically Dialog Read from File
		Lines	Line Polyline Arc Circle Spline
		Surfaces	Rectangle Graphically Planar Quadrangle Rotary Pipe B-Spline
		Openings	Graphically Dialog
		Thicknesses	Graphically Dialog
		Solids	Graphically - Block Layered Solid

			General Solid
	FE-Mesh Refinement	Graphically	
		Dialog	
	Domain Properties	Material Distribution	
		Root Distribution	
		Nodal Recharge	
		Scaling Factor	Hydraulic Conductivity
			Pressure Head
			Water Content
		Local Anisotropy	Angle
			First Component
			Second Component
			Index
		Subregions	
		Observation Nodes	
		Drains	
		Flowing Particles	
	Initial Conditions	Pressure Head/Water Content	
		Concentration	
		Nonequilibrium Concentration	
		Temperature	
		Import	
	Boundary Conditions	Water Flow	No Flux
			Constant Head
			Constant Flux
			Seepage Face
			Variable Head 1-4
			Variable Flux 1-4
			Free Drainage
			Deep Drainage
			Atmospheric Boundary
		Solute Transport	First-Type
			Third-Type
			Volatile Type
		Heat Transport	First-Type
			Third-Type
	Cross-Sections	Graphically	
		Dialog	
	Mesh Line	Graphically	
		Dialog	
	Auxiliary Objects	Dimension	
		Comment	
		Bitmap	
		Background Layer	
E Calculation	FE-Mesh Parameters		
	Generate FE-Mesh		
	Delete FE-Mesh		
	FE-Mesh Statistics		
	Advance FE-Mesh Generation	Fundamental Triangulation	
		Mesh Refinement	
		Retriangulation	
		Check of Convexity	
		Mesh Smoothing	
	Calculate Current Project		
	Calculate All Open Projects		

Select Projects to Calculate

F Results

- Display Quantity
  - Pressure Heads
  - Water Content
  - Concentration
  - Nonequilibrium Concentration
  - Temperature
  - Velocity
- Boundary Information
  - Pressure Heads
  - Boundary Fluxes
  - Cumulative Fluxes
  - Solute Fluxes
- Observation Points
- Soil Hydraulic Properties
- Run Time Information
- Mass Balance Information
- Chemical Mass Balance Information
- Convert Output to ASCII
- Inverse Solution Results
- Fluxes across Mesh Lines
- Time Layer
  - First
  - Last
  - Previous
  - Next
  - Animation
- Charts
  - Cross-Section
  - Boundary Line
  - Mesh-Line
- Flowing Particles
  - Draw Particles Positions
  - Draw Particles Trajectories
- Delete Results

G Tools

- Show Grid
- Snap to Grid
- Grid and Work Plane
- Define Work Plane
  - Set Origin
  - Define XY
  - Define YZ
  - Define XZ
- Coordinate System
- Color Scale
  - Color Smoothing
  - Min/Max Values Global in Time
  - Min/Max Values Global in Space
  - Standard Scale
  - Custom Scale
  - Edit Scale
- Translate
- Rotate
- Mirror
- Stretch
- Skew
- Intersect Lines
- Intersect Surfaces
- Split Lines
  - Graphically
  - n Points
  - Distance

	Insert Points on Line	Graphically n Points Distance
	Check Data Consistency	
	Repair Geometry	
	Generate Domain Surfaces	
	Create Video File	
H Options	Rendering Mode	Solid Model Transparent Model Wire Frame Model
	Graph Type	Isolines Colormaps Isosurfaces Color Points Color Edges Velocity Vectors
	Display Options	Edit Default Read Save As
	Program Options	
I Windows	New Window	
	Arrange Symbols	
	Main and Secondary	
	Tile Horizontally	
	Tile Vertically	
	Cascade	
	Close All	
J Help	Context Sensitive Help	
	Help – Contents and Index	
	Hydrus User Manual	
	Hydrus Technical Manual	
	Hydrus Online	
	Troubleshooting	
	Hydrus License and Activation	
	About Hydrus	

Table 26. Brief description of HYDRUS menu commands.

Group	Command	Brief description of the command
A	**File**	
	New	Creates a new project after user provides required information (name and description) in the **New Project** dialog window (Fig. 4). Project will be located in the current Project Group.
	Open	Opens an existing project (represented by the *project_name*.h3d2 file) using the **Open** dialog window, which a user uses to browse for the HYDRUS project.
	Close	Closes an open project.
	Save	Saves the input data of an actual project specified in the main program module if the data were either newly created or changed during an application run.
	Save As	Saves data of a particular project under a new project name using **Save As** dialog window.
	Save All	Saves data of all projects.
	Import and Export	
	Import Hydrus-2D Project	Imports Hydrus-2D projects from Version 2.0.
	Import Input Data from *.IN Files	Imports input data from *.in files that may have been modified manually outside of the HYDRUS GUI.
	Import Input Data from another HYDRUS Project	Imports data from another project and interpolates properties when FE-Mesh grids are different.
	Export Data for Hydrus Solver	Exports data for the HYDRUS solver into the working directory from which the computational module reads inputs and into which it writes outputs.
	Export Data to ParSWMS	ParSWMS is a parallelized version of SWMS-3D, which can be run on clusters or supercomputers. This commands creates input files for ParSWMS from the HYDRUS project.
	Read Points from a Text File	Reads single point coordinates from a text file.
	Import Geometry from a Text File	Reads definition of the entire geometry from a text file.
	Import Geometry from a DXF File	Reads definition of the entire geometry from a DXF file.
	Import Geometry from a TIN File	Reads definition of the entire geometry from a TIN file.
	Export Geometry from a Text File	Writes definition of the entire geometry to a text file.
	Export only Selected Objects	Writes definition of the selected objects to a text file.
	Imports Data from ParSWMS	Imports output data created by ParSWMS on a supercomputer or cluster of computers and display them in HYDRUS GUI.
	Print	Prints the content of the View window.
	Print Preview	Previews the content of the View window before printing.
	Print to the Clipboard	Copies the content of the View window to the clipboard for subsequent pasting into other software packages.
	Print Options	Select various print options, such as print quality, text size, frame, and text content (Fig. 170).
	Print Setup	Selects a printer and printer connection.
	Project Information	Displays information about the current project (in the **General Data** dialog window (Fig. 4)).
	Project Manager	Calls the **Project Manager** (Figs. 2 and 3) to manage data of existing projects; helps to locate, open, copy, delete or rename the desired projects and their data.

Recent Files	Displays recently opened projects.
Exit	Closes open projects and leaves the program. This command informs users before exiting the application whether or not the input data of open projects were changed during the application run. If changes did occur, users are given an option to save data before exiting the application.

B Edit

Undo	Reverses the last edit action.
Redo	Repeats the last edit action.
Copy	Copies a selected object.
Paste	Pastes a selected object.

Select

Select by Rhomboid	Selects objects by means of a rhomboid.
Select by Circle	Selects objects by means of a circle.
Select by Polygon	Selects objects by means of a polygon.
Add to Selection	Add new object to existing selection
Remove from Selection	Remove objects from existing selection
Standart Selection Mode	Selects objects by means of a qvadrilateral.
Properties	Displays properties of a selected object.
Find	Finds an object.
Delete	Deletes a selected object.
Delete All	Deletes all objects.

Domain Geometry

Domain Type and Units	Specifies whether the flow and transport problem occurs in a two- or three-dimensional transport domain, and whether the domain is simple or complex using the **Domain Type and Units** dialog window (Fig. 6).
Simple Domain	Specifies parameters (dimensions and slopes) for simple rectangular or hexahedral transport domains using the **Rectangular** (Fig. 10) or **Hexahedral Domain Definition** (Fig. 11) dialog windows.
3D-Layered Domain	Calls Edit 3D-Layered Domain dialog window for editing the object.
Delete 3D-Layered Domain	Deletes 3D-Layered Domain.
Points	Edits selected points.
Lines	Edits selected lines using the **Edit Curve** dialog window (Fig. 46).
Surfaces	Edits selected surfaces.
Openings	Edits selected openings.
Thickness Vectors	Edits selected thickness vectors.
Solids	Edits solids.

Flow Parameters

Main Processes	Selects the processes to be simulated, i.e., water flow, multiple solute transport, heat transport, and/or root water uptake (the **Main Processes** dialog window (Fig. 12)).
Inverse Solution	Selects type of weighting of measured data, and whether soil hydraulic parameters, solute transport parameters, and/or heat transport parameters, are to be fitted (the **Inverse Solution** dialog window (Fig. 13)).
Time Information	Selects time units, and gives the time discretization information (the **Time Information** dialog window (Fig. 15)).

Output Information	Specifies print options (The **Output Information** dialog window (Fig. 16)).
Water Flow Parameters	
Iteration Criteria	Specifies iteration criteria for the solution precision and parameters for the time step control (The **Iteration Criteria** dialog window (Fig. 17)).
Hydraulic Properties Model	Selects the type of model used for the soil hydraulic properties, and decides whether hysteresis is to be considered (the **Soil Hydraulic Model** dialog window (Fig. 18)).
Soil Hydraulic Parameters	Specifies parameters in the soil hydraulic model (the **Water Flow Parameters** dialog window (Fig. 19)).
Anisotropy Tensors	Defines anisotropy tensors for three-dimensional applications (the **Tensors of Anisotropy** dialog window (Fig. 22)).
Solute Transport Parameters	
General Information	Selects the time and spatial weighting schemes for numerical solution of the solute transport equation; specifies the number of solutes to be considered (the **Solute Transport** dialog window (Fig. 23)).
Solute Transport Parameters	Specifies solute transport parameters (the **Solute Transport Parameters** dialog window (Fig. 25)).
Solution Composition	Specifies solution, adsorbed, and precipitated concentration combinations for the UNSATCHEM module (the **Solution Compositions** dialog window (Fig. 30)).
Solute Reaction Parameters	Specifies solute reaction parameters (the **Solute Reaction Parameters** dialog window (Fig. 26)).
Constructed Wetlands Parameters I	Specifies parameters for constructed wetlands (the **Constructed Wetland Model Parameters I** dialog windows (Fig. 38)).
Constructed Wetlands Parameters II	Specifies parameters for constructed wetlands (the **Constructed Wetland Model Parameters II** dialog windows (Fig. 40)).
Temperature Dependence	Specifies parameters defining the temperature dependence of reaction and transport parameters (the Temperature Dependent Solute Transport and Reaction Parameters dialog window shown in Figure 28).
Water Content Dependence	Specifies parameters defining the water content dependence of reaction parameters (the Water Content Dependent Solute Reaction Parameters dialog window shown in Figure 29).
Chemical Parameters	Specifies various chemical parameters and selections for the UNSATCHEM module (the **Chemical Parameters** dialog window (Fig. 31)).
Fumigant Application	Allows additional application of a specified mass of a chemical into the transport domain (a specified location) at specified time.
Heat Transport Parameters	Specifies heat transport parameters (the **Heat Transport** dialog window; Fig. 32).
Root Water Uptake	
Root Water Uptake Models	Selects the root water uptake stress response models for both salinity and water stress (the **Root Water Uptake Model** dialog window, Fig. 33).
Pressure Head Reduction	Specifies parameters in the root water uptake water stress response model (the **Root Water Uptake Parameters** dialog window; Fig. 34).
Osmotic Head Reduction	Specifies parameters in the root water uptake salinity stress response model (the **Root Water Uptake Parameters** dialog window; Fig. 35).

Variable Boundary Condition	Specifies time-dependent boundary conditions for all transport processes (the **Time Variable Boundary Conditions** dialog window; Fig. 37).
Data for Inverse Solution	Specifies data for the inverse solution, their type, location and associated weight (the **Data for Inverse Solution** dialog window; Fig. 14).

FE-Mesh

FE-Mesh Generator	Selects the structured or unstructured finite element mesh generator (the **Finite Element Mesh Generator** dialog window; Fig. **Error! Bookmark not defined.**).
FE-Mesh Parameters	Specifies either parameters of the Unstructured Finite Element Mesh Generator (the **FE-Mesh Parameters** dialog window; Figs. 92 through 95) or parameters of the structured mesh (the **Rectangular Domain Discretization** dialog window (Fig. 90) or the **Hexahedral Domain Discretization** dialog window (Fig. 91)).
Generate FE-Mesh	Generates unstructured finite element mesh.
Delete FE-Mesh	Deletes unstructured finite element mesh.
Remove Selected FE-Elements	Removes selected finite elements from the finite element mesh. Note that this operation should not be performed when properties are specified on Geometric Objects.
FE-Mesh Statistics	Provides information about finite element mesh (the **FE-Mesh Information** dialog window (Fig. 104).
Select Mesh Nodes	Selects FE-Mesh nodes. This command is usually used to select nodes that are then either used to define the new FE-Mesh Section or removed from the FE-Mesh.
Select Mesh Elements	Selects FE-Mesh elements (to perform similar operations as for selected mesh nodes).

Advanced FE-Mesh Generation

Fundamental Triangulation	Performs triangulation of boundary nodes based on the Delaunay criterion.
Mesh Refinement	Inserts a new point in the center of all triangles that do not fulfill the smoothness criterion.
Retriangulation	Retriangulates mesh according to Delaunay criterion.
Check of Convexity	Corrects possible errors which may appear during smoothing and retriangulating.
Mesh Smoothing	Smoothes the mesh by solving a set of coupled elliptic equations using a recursive algorithm.

Domain Properties

Material Distribution	Specifies the spatial distribution of soil materials.
Root Distribution	Specifies the spatial distribution of root water uptake.
Nodal Recharge	Specifies the spatial distribution of nodal recharge.

Scaling Factor

Hydraulic Conductivity	Specifies the spatial distribution of hydraulic conductivity scaling factors.
Pressure Head	Specifies the spatial distribution of pressure head scaling factors.
Water Content	Specifies the spatial distribution of water content scaling factors.

Local Anisotropy

Angle	Specifies the spatial distribution of the angle of local anisotropy.
First Component	Specifies the spatial distribution of the first component of local anisotropy.
Second Component	Specifies the spatial distribution of the second component of local anisotropy.

Index	Specifies the spatial distribution of the index that represents the local anisotropy tensor.
Subregions	Specifies the spatial distribution of subregions for the mass balance calculations.

Observation Nodes

Edit	Specifies observation nodes for output of the pressure head, water content, temperature, and concentration at each time step.
Delete	Deletes selected observation nodes.
Clear All	Deletes all observation nodes.

Drains

Edit	Specifies nodal points representing tile drains.
Delete	Deletes selected tile drains.
Clear All	Deletes all tile drains.
Drain Parameters	Specifies drain parameters.

Flowing Particles

Edit	Specifies nodal points representing flowing particles.
Delete	Deletes selected flowing particles.
Clear All	Deletes all flowing particles.

Stochastic Distribution of S.F.	Generates a stochastic distribution of scaling factors.
Subregions = Material Distribution	Makes the subregions for mass balance calculations similar to those for the soil materials.
Nonequilibrium Conc. = a * Equil. Conc.	Specifies that nonequilibrium concentrations (i.e., kinetically sorbed concentrations or concentrations in the immobile water) are a multiple of the liquid phase concentrations.
Parameters for Root Distribution	Specifies parameters for the spatial distribution of root water uptake.
Delete All Domain Properties	Command used when defining properties on Geometrical Objects. Deletes all defined domain properties and assigns default values.
Default Domain Parameters	Specifies default domain properties that are constant for the same depths (the **Default Domain Properties** dialog window; Fig. 106).

Initial Conditions

Pressure Head/Water Content	Specifies the initial condition for water flow.
Concentration	Specifies the initial condition for solute transport (equilibrium concentrations).
Nonequilibrium Concentration	Specifies the initial condition for solute transport (nonequilibrium concentrations).
Temperature	Specifies the initial condition for heat transport.
Import	Imports the initial condition from previous simulations for water flow, and solute and heat transport.
Delete All Initial Conditions	Command used when defining Initial Conditions on Geometrical Objects. Deletes all defined Initial Conditions and assigns default values.

Boundary Conditions

Water Flow	Specifies boundary conditions for water flow.
Solute Transport	Specifies boundary conditions for solute transport.
Heat Transport	Specifies boundary conditions for heat transport.
Boundary Conditions Options	Specified additional system-dependent water flow boundary conditions.
Deletes All Boundary Conditions	Clears all boundary conditions and assigns a No Flow boundary condition on all boundaries

Properties and Conditions on FE-Mesh	Selects that spatially variable properties (e.g., materials, initial conditions) are assigned directly to the FE-Mesh rather than to Geometrical Objects

Model Sections

Edit Sections	Calls the FE-Mesh Section dialog (Fig. 105). HYDRUS recognizes two different definitions of Sections – one for geometrical objects and one for the FE-mesh. A different dialog appears when called from the "Domain Geometry" part of the program. In all other cases, the FE-mesh Section dialog appears.
Generate Sections	Generates Geo-Sections and FE-Mesh Sections.
New Section from Selection	Creates a new section from currently selected objects/FE-Mesh
New Section from View	Creates a new section from currently displayed objects/FE-Mesh
Display Whole Domain	Displays all objects or entire FE-Mesh
Display Previous	Displays a previously displayed view (sections)
Hide Selection	Hides selected elements.
Display only Selection	Displays only currently selected objects/FE-Mesh
Display Reverse	Hides currently displayed objects/FE-Mesh and displays currently hidden objects/FE-Mesh
Cut with Rectangle	Displays objects/FE-mesh nodes within a certain rectangle or rhomboid and hides all the others
Cut with Indexes	Displays objects with given indexes and hides all the others
Import FE-Mesh Sections	Import FE-Mesh Sections

Cross-Sections

Edit	Edits a cross-section
Delete Selected	Deletes selected cross-sections
Delete All	Deletes all cross-sections
Auto-Adjust Work Plane	Adjust Work Plane

Auxiliary Objects

Dimensions

Delete Selected	Deletes selected dimensions
Delete All	Deletes all dimensions

Comments

Edit	Edits a comment
Delete Selected	Deletes selected comments
Delete All	Deletes all comments

Background Layers	Geometrical objects that are imported to HYDRUS and are used as templates for defining HYDRUS geometries
Edit	Edits a selected Background Layer
Move	Moves a selected Background Layer
Rotate	Rotates a selected Background Layer
Mirror	Mirrors a selected Background Layer
Stretch	Stretches a selected Background Layer
Skew	Skews a selected Background Layer
Delete All	Deletes all Background Layers

C View

Geometry	Sets the View window to View/Edit Domain Geometry mode.
FE Mesh	Sets the View window to View/Edit FE-Mesh mode.
Domain Properties	Sets the View window to View/Edit Domain Properties mode, to edit materials.
Initial Conditions	Sets the View window to View/Edit Initial Conditions mode, to edit pressure head initial conditions.

Boundary Conditions	Sets the View window to View/Edit Boundary Conditions mode, to edit water flow boundary conditions.
Results	Sets the View window to View Results mode, to view pressure head distribution.
Navigator	Displays or hides the Navigator window.
Edit Bar	Displays or hides the Edit Bar.
Tabs in View	Displays or hides Tabs in the View window.
Status Bar	Displays or hides the Status Bar.
Toolbars	Selects which toolbars are to be displayed (the **Toolbars** dialog window, Fig. 144).
Arrange Toolbars	Arranges toolbars.
Customize Toolbars	Customizes toolbars (the **Customize Toolbars** dialog window, Fig. Fig. 145).
Standard View	Sets a default viewing direction (in 3D) and performs the "View All" command
Zoom by Rectangle	Zooms in on a certain part of the View window using a rectangle.
View All	Changes a scroll position and a zoom factor so that all currently displayed objects are visible in the View Window. This command does not change the viewing direction.
Previous View	Shows the previous view on a certain part of the View window.
Dynamic View (Scroll, Zoom, Rotate)	Sets the View windows so that dynamic actions can be carried out with a cursor. Moving the cursor while holding the left mouse button allows the object to be displayed in a different part of the View window. Pressing the Shift button on the keyboard allow zooming actions around the cursor.
View Stretching	Calls the View Stretching Factors dialog window (Fig. 136) and adjust stretching factors.
Perspective	Sets perspective view.
Auto-Rotate	Starts *Autorotate* function that will rotate the transport domain in the View window.
Cancel Partial View	Cancels the **Partial View** displays the entire transport domain.

View in Direction

Isometric	Sets isometric view.
In X-direction	Sets the view of the transport domain in the *X*-direction.
In Y-direction	Sets the view of the transport domain in the *Y*-direction.
In Z-direction	Sets the view of the transport domain in the *Z*-direction.
Reverse X-direction	Sets the view of the transport domain in the reverse *X*-direction.
Reverse Y-direction	Sets the view of the transport domain in the reverse *Y*-direction.
Reverse Z-direction	Sets the view of the transport domain in the reverse *Z*-direction.
List Boxes for Inverse Data	Shows text information in the inverse data list (the **Data for Inverse Solution** dialog window; Fig. 14).

D Insert

Domain Geometry

Points

Graphically	Inserts single points graphically.
Dialog	Inserts single points numerically (the **Edit Point** dialog window without the FE-Mesh tab; Fig. 44).

Lines

Line	Inserts a line either graphically or numerically (the **Edit Curve** dialog window without the FE-Mesh tab; Fig. 46).

Polyline	Inserts a polyline either graphically or numerically (the **Edit Curve** dialog window without the FE-Mesh tab; Fig. 46).
Arc	Inserts an arc either graphically or numerically.
Circle	Inserts a circle either graphically or numerically.
Spline	Inserts a spline either graphically or numerically (the **Edit Curve** dialog window without the FE-Mesh tab; Fig. 46).
Surfaces	Inserts a surface either graphically or numerically.
Planar Surface	Inserts a planar surface either graphically or numerically.
Quadrangle Surface	Inserts a Quadrangle surface either graphically or numerically.
Rotary Surface	Inserts a Rotary surface either graphically or numerically.
Pipe Surface	Inserts a Pipe surface either graphically or numerically.
B-Spline Surface	Inserts a B-Spline surface either graphically or numerically.
Openings	Inserts an opening either graphically or numerically.
Thicknesses	Inserts thicknesses either graphically or numerically.
Solids	Inserts solids either graphically or numerically.
Layered Solid	Inserts Layered solids either graphically or numerically.
General Solid	Inserts General solids either graphically or numerically.

FE-Mesh Refinement

Graphically	Inserts new FE-mesh refinement graphically (the **FE-Mesh refinement** dialog window; Fig. 97).
Dialog	Defines new FE-mesh refinement graphically (the **FE-Mesh refinement** dialog window; Fig. 97).

Domain Properties

Material Distribution	Specifies the spatial distribution of soil materials.
Root Distribution	Specifies the spatial distribution of root water uptake.
Nodal Recharge	Specifies the spatial distribution of nodal recharge.

Scaling Factor

Hydraulic Conductivity	Specifies the spatial distribution of the hydraulic conductivity scaling factors.
Pressure Head	Specifies the spatial distribution of the pressure head scaling factors.
Water Content	Specifies the spatial distribution of the water content scaling factors.

Local Anisotropy

Angle	Specifies the spatial distribution of the angle of local anisotropy (for two-dimensional applications).
First Component	Specifies the spatial distribution of the first component of local anisotropy (for two-dimensional applications).
Second Component	Specifies the spatial distribution of the second component of local anisotropy (for two-dimensional applications).
Index	Specifies the spatial distribution of anisotropy tensors (for three-dimensional applications).
Subregions	Specifies the spatial distribution of subregions for mass balance calculations.
Observation Nodes	Specifies observation nodes for output of the pressure head, water content, temperature, and concentration at each time step.
Drains	Specifies nodal points representing tile drains.
Flowing Particles	Specifies nodal points representing flowing particles.

Initial Conditions

Pressure Head/Water Content	Specifies the initial condition for water flow.
Concentration	Specifies the initial condition for solute transport.
Nonequilibrium Concentration	Specifies the initial condition for nonequilibrium solute transport.
Temperature	Specifies the initial condition for heat transport.

Import	Imports initial conditions for water flow, solute transport, and/or heat transport.

Boundary Conditions

Water Flow

No Flux	Specifies a no-flux boundary condition along a selected part of the boundary.
Constant Head	Specifies a constant pressure head boundary condition along a selected part of the boundary.
Constant Flux	Specifies a constant flux boundary condition along a selected part of the boundary.
Seepage Face	Specifies a seepage face boundary condition along a selected part of the boundary.
Variable Head 1-4	Specifies a variable pressure head boundary condition along a selected part of the boundary.
Variable Flux 1-4	Specifies a variable flux boundary condition along a selected part of the boundary.
Free Drainage	Specifies a free drainage boundary condition along a selected part of the boundary.
Deep Drainage	Specifies a deep drainage boundary condition along a selected part of the boundary.
Atmospheric Boundary	Specifies an atmospheric boundary condition along a selected part of the boundary.

Solute Transport

First-Type	Specifies a first-type boundary condition for solute transport along a selected part of the boundary.
Third-Type	Specifies a third-type boundary condition for solute transport along a selected part of the boundary.
Volatile Type	Specifies a volatile-type boundary condition for solute transport along a selected part of the boundary.

Heat Transport

First-Type	Specifies a first-type boundary condition for heat transport along a selected part of the boundary.
Third-Type	Specifies a third-type boundary condition for heat transport along a selected part of the boundary.

Cross-Sections

Graphically	Inserts a cross-section graphically.
Dialog	Inserts a cross-section using the dialog window.

Mesh Line

Graphically	Inserts a mesh line graphically.
Dialog	Inserts a mesh line using the dialog window.

Auxiliary Objects

Dimension	Inserts auxiliary object (dimensions).
Comment	Inserts auxiliary object (comment).
Bitmap	Inserts auxiliary object (bitmap).
Background Layer	Inserts auxiliary object (background layer).

E Calculation

FE-Mesh Parameters	Specifies either parameters of the Unstructured Finite Element Mesh Generator (the **FE-Mesh Parameters** dialog window; Figs. 92 through 95) or parameters of the structured mesh (the **Rectangular Domain Discretization** dialog window (Fig. 90) or the **Hexahedral Domain Discretization** dialog window (Fig. 91)).
Generate FE-Mesh	Generates the unstructured finite element mesh.

Delete FE-Mesh	Deletes the unstructured finite element mesh.
FE-Mesh Statistics	Provides information about the finite element mesh (the **FE-Mesh Information** dialog window (Fig. 104).

Advanced FE-Mesh Generation

Fundamental Triangulation	Performs triangulation of boundary nodes based on the Delaunay criterion.
Mesh Refinement	Inserts a new point in the center of all triangles that do not fulfill the smoothness criterion.
Retriangulation	Retriangulates mesh according to Delaunay criterion.
Check of Convexity	Corrects possible errors which may appear during smoothing and retriangulating.
Mesh Smoothing	Smoothes the mesh by solving a set of coupled elliptic equations using a recursive algorithm.

Calculate Current Project	Carries out calculations for the currently active project.
Calculate Current Project	Carries out calculations for all currently open projects.
Select Projects to Calculate	Opens the Project Manager to select projects to be calculated.

F Results

Display Quantity

Pressure Head	Displays results in terms of pressure heads.
Water Content	Displays results in terms of water contents.
Velocity	Displays results in terms of velocities.
Concentration	Displays results in terms of concentrations
Nonequilibrium Concentration	Displays results in terms of nonequilibrium concentrations (kinetically sorbed or in the immobile water)
Temperature	Displays results in terms of temperatures

Boundary Information

Pressure Heads	Graphical presentation of pressure heads at different boundaries and in the root zone.
Boundary Fluxes	Graphical presentation of potential and actual boundary water fluxes at different boundaries.
Cumulative Fluxes	Graphical presentation of potential and actual cumulative boundary water fluxes.
Solute Fluxes	Graphical presentation of actual and cumulative boundary solute fluxes.
Observation Points	Graphical presentation of changes in water content, pressure head, temperature, and/or solute and sorbed concentration at specified observation nodes.
Soil Hydraulic Properties	Graphical presentation of the soil hydraulic properties.
Run Time Information	Graphical presentation of information about the number of iterations, time step, and Peclet and Courant numbers.
Mass Balance Information	Displays mass balance information and mean profile properties.
Chemical Mass Balance Information	Displays chemical mass balance information.
Convert Output to ASCII	Convert binary input and output files into ASCII files.
Inverse Solution Results	Displays information about the inverse solution.
Fluxes across Mesh Lines	Displays actual and cumulative, water and solute fluxes across selected mesh lines.

Time Layer

First	Displays a particular variable at the first time layer.
Last	Displays a particular variable at the last time layer.
Previous	Displays a particular variable at the previous time layer.

Next	Displays a particular variable at the next time layer.
Animation	Displays time layers of a particular variable consecutively and continuously.

Charts

Cross-Section	Displays values of a particular variable along an arbitrary cross-section.
Boundary Line	Displays values of a particular variable along a certain part of a boundary.
Mesh Line	Displays values of a particular variable along a selected mesh line.

Flowing Particles

Draw Particles Positions	Draws positions of flowing particles.
Draw Particles Trajectories	Draws trajectories of flowing particles.

Delete Results	Deletes all output results.

G Tools

Show Grid	Shows or hides the grid.
Snap to Grid	Specifies whether or not the mouse should move in steps defined by the grid.
Grid and Work Plane	Calls the **Grid and Work Plane** dialog window (Fig 135).

Define Work Plane

Set Origin	Redefines origin of the grid.
Define XY	Sets Work Plane to the XY plane.
Define YZ	Sets Work Plane to the YZ plane.
Define XZ	Sets Work Plane to the XZ plane.

Coordinate System	Selects coordinate system

Color Scale

Color Smoothing	Changes color from abrupt to gradual at isolines.
Min/Max Values Global in Time	Selects minimal and maximal values for the color scale either for the entire time duration or only for a selected time layer.
Min/Max Values Global in Space	Selects minimal and maximal values for the color scale either for the entire transport domain or only for displayed part of the domain.
Standard Scale	Selects a standard color scale for the display of a particular variable.
Custom Scale	Selects a custom color scale for the display of a particular variable.
Edit Scale	Calls the **Edit Isoband Value and Color Spectra** dialog window (Fig 127).

Translate	Moves or copies a selected object.
Rotate	Rotates a selected object.
Mirror	Mirrors a selected object.
Stretch	Stretches a selected object.
Skew	Skews a selected object.

Intersect Lines	Finds the intercept of two lines and insert an interception point on the lines.
Intersect Surfaces	Finds the curve that is created by the intercept of two surfaces.
Split Lines	Splits lines.
Insert Points on Line	Inserts points on a line.

Check Geometry	Checks geometry for consistency.
Repair Geometry	Repairs geometry if inconsistent
Generate Domain Surfaces	Attempts to generate Domain Surface if they were not specified.

Create Video File	Allows users to save flow animation in a video file.

H Options

Rendering Mode

Solid Model	Displays the transport domain as a solid object.
Transparent Model	Displays the transport domain as a transparent object.
Wire Frame Model	Displays the transport domain as a wired object.

Graph Type

Isolines	Displays the spatial distribution of a particular variable by means of isolines.
Colormaps	Displays the spatial distribution of a particular variable by means of isobands.
Isolines	Displays the spatial distribution of a particular variable by means of isosurface.
	Color Points Displays the spatial distribution of a particular variable by means of color points.
Color Edges	Displays the spatial distribution of a particular variable by means of color edges.
Velocity Vectors	Displays Darcy velocity vectors.

Display Options

Edit	Edits display options in the **Display Options** dialog window (Fig 126).
Default	Sets display options to their default values.
Read	Reads display options from a file.
Save As	Saves display options to a file.
Program Options	Displays program options information (the **Program Options** dialog window has two tabs, one related to **Graphics** (Fig. 149) and one to **Program** itself (Fig. 150)).

I Windows

New Window	Open a new View window.
Arrange Symbols	Arranges minimized windows as icons at the bottom of the **View** window.
Main and Secondary	Displays open View windows as main and secondary windows.
Tile Horizontally	Tiles open View windows horizontally.
Tile Vertically	Tiles open View windows vertically.
Cascade	Cascades open View windows.
Close All	Closes all open View windows.

J Help

Context Sensitive Help	Help for various objects of GUI.
Help – Contents and Index	Displays help information.
Hydrus User Manual	Displays a PDF version of the HYDRUS User Manual
Hydrus Technical Manual	Displays a PDF version of the HYDRUS Technical Manual
Hydrus Online	Launches Internet Explorer Browser and opens the HYDRUS web page
Troubleshooting	Launches Internet Explorer Browser and opens the Troubleshooting page of the HYDRUS web page
Hydrus License and Activation	Displays the Hydrus license and activation information (the **HYDRUS License and Activation** dialog window; Fig. 153).
About Hydrus	Displays the version and authors of the HYDRUS application.

9. Miscellaneous Information

9.1. *Program Options*

The **Program Options** dialog window has four tabs, one related to **Graphics** (Fig. 149), one to **Program Options** (Fig. 150), one to **FE-Mesh** (Fig. 151), and one to **Files and Directories** (Fig. 152).

On the left side of the **Graphics** Tab (*OpenGL*) one can turn on or off the *OpenGL Hardware Acceleration* (OpenGL is a library of functions developed by Silicon Graphics Inc. for handling graphical objects), and select the speed for *OpenGL optimization*.

On the right side of the **Graphics** Tab (*Options*) one can select

a) *Simplified display in Move modus*
b) whether or not an object is selected when the cursor hovers above it (*Pre-selection (Mark object while hovering above it with cursor)*),
c) whether or not values and properties are displayed numerically when the cursor is close to a selected object (*Display values/properties at pre-selected objects*),
d) a different background (*Gradient Background*) (visually more effective background is displayed, which may be useful for presentations), and
e) minimum time for one frame during flow animation.

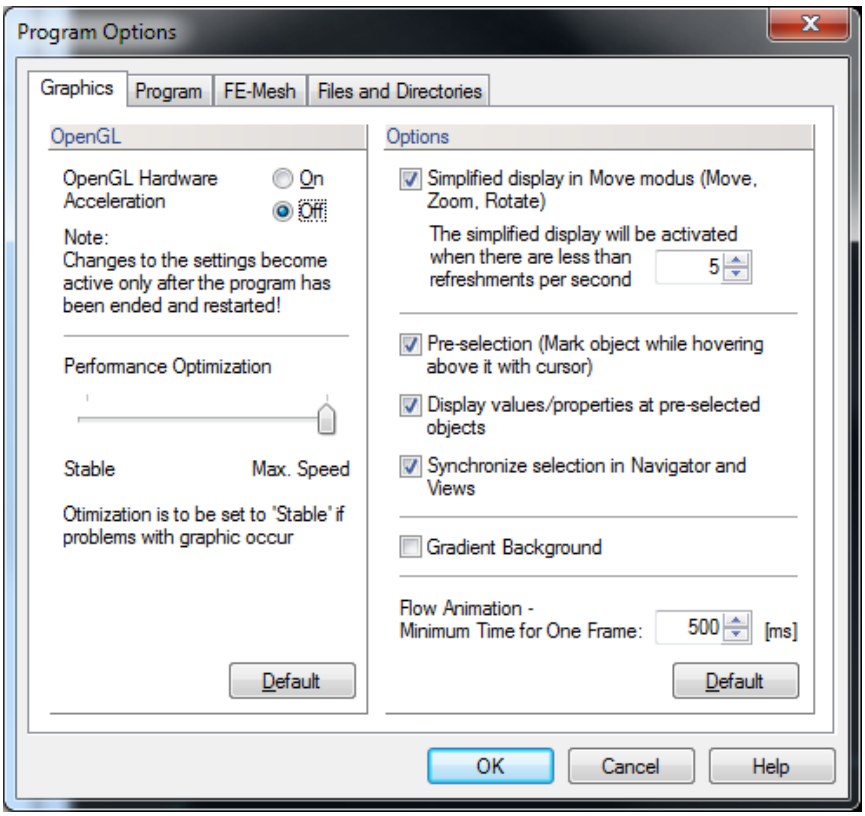


Figure 149. The Program Options dialog window (the Graphics Tab).

Simplified Display Mode: When the graphics (View Window update) is too slow, this option accelerates it during dynamic rotating, moving or zooming. When rotating the model, only its simplified version is drawn, which results into faster display of the model. When rotating is finished, the full model is displayed again. This option is initiated only when the number of "refreshments" per second falls below the specified number.

When the checkbox "**Synchronize selection in the Navigator and Views**" is checked, clicking on any object on the **Navigator Bar** leads to its automatic selection in Views. When this checkbox is not checked, one can select an object by clicking on it with the right mouse button at the **Navigator Bar** and using the **Select** command from the popup menu.

In the **Undo and Autosave** part of the **Program Options** Tab (*Options*) one can

a) select a time interval for *Auto-save*
b) specify *Memory size for the Undo buffer*, and

In the **General Options** part of the **Program Options** Tab (*Options*) one can

a) specify whether or not the program *Reloads last opened projects at startup*
b) specify whether or not the program should *Save automatically windows settings on close project*

In the **Calculation and Results** part of the **Program Options** Tab (*Options*) one can

a) specify whether the results are to be kept in an external directory (*By default keep results in external directory*),
b) select whether the FE-Mesh is to be saved in text format (*Save FE-Mesh in text format*),
c) select whether or not Domain Properties are to be saved in text format (*Save Domain Properties in text format*).

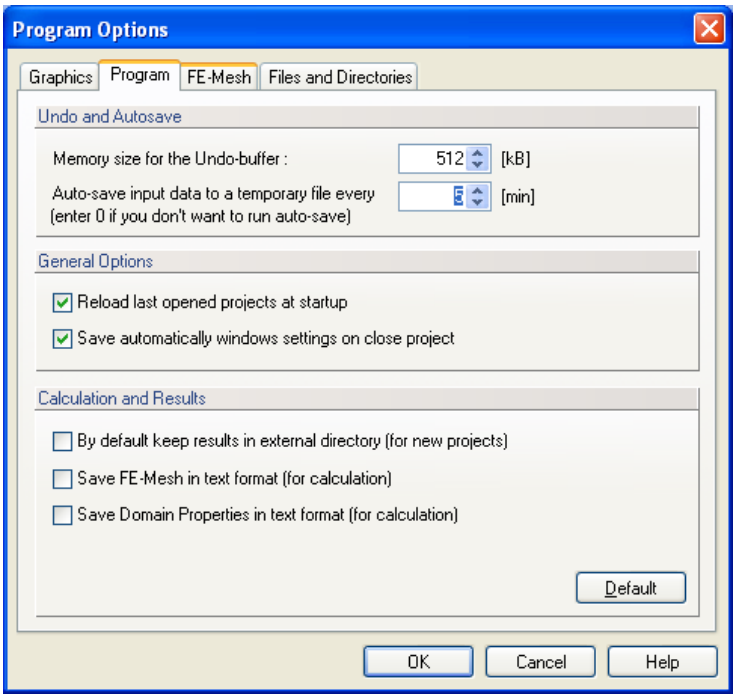


Figure 150. The Program Options dialog window (the Program Options Tab).

In the **Mesh Limits** part of the **FE-Mesh** Tab (*Options*) one can

a) specify the *Recommended maximum number of finite elements for 2D projects,*
b) specify the *Recommended maximum number of finite elements for 3D projects.*

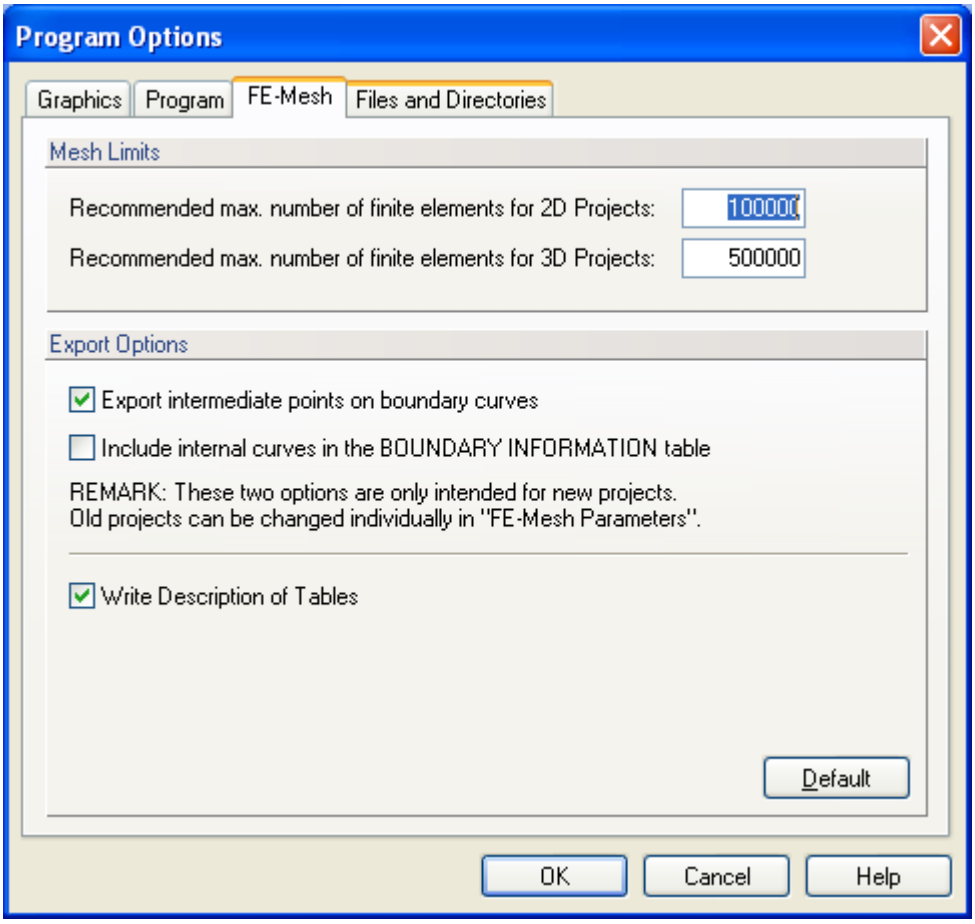


Figure 151. The FE-Mesh Options dialog window (the Program Options Tab).

In the **Files and Directories** Tab (*Options*) one can specify locations of various HYDRUS files and the file having information about display options:

- Directory for HYDRUS Settings and Authorization Files
- Working Directory for Temporary Files
- Default Directory for HYDRUS Projects
- Configuration file for display options

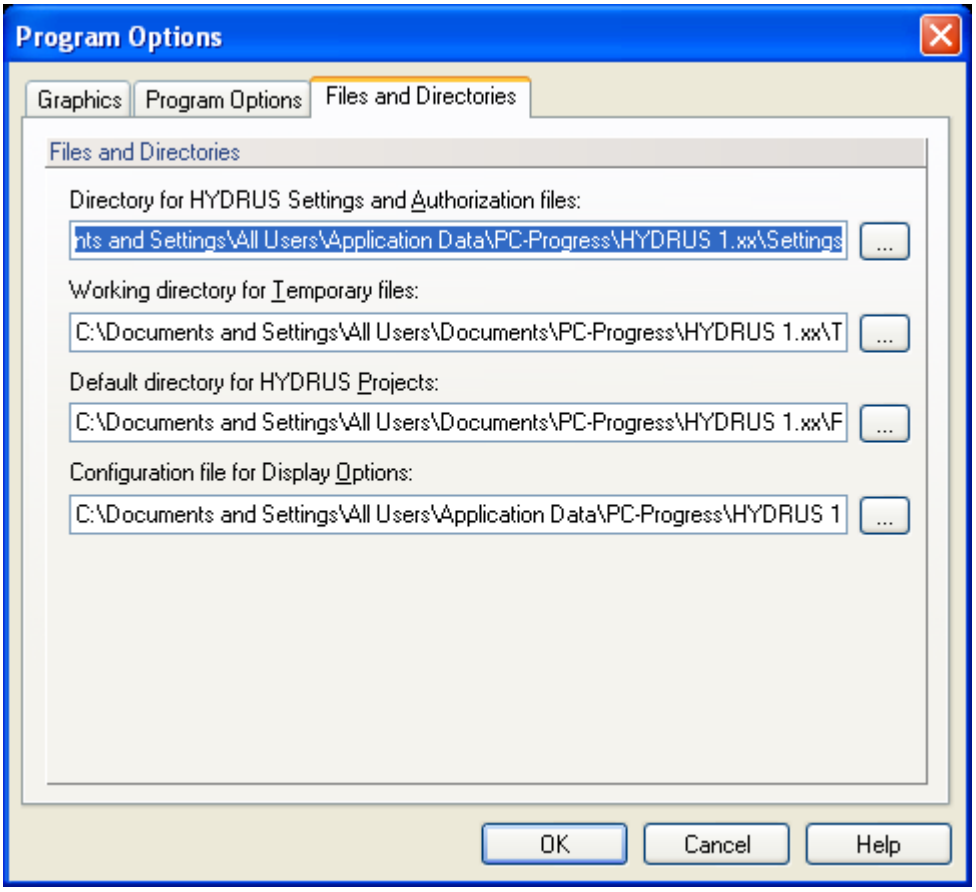


Figure 152. The Program Options dialog window (the Program Directories Tab).

9.2. HYDRUS License and Activation

HYDRUS is protected by a software lock that is based on information about the hardware on which it is run. Without activation HYDRUS works as a demo version - you can run it but you will not be able to run calculations and save your data. A customer can choose to **Activate** HYDRUS **by E-mail** with the help of the HYDRUS support or directly **On-line** (an internet connection is required). Using the **Online** activation system, customers can themselves manage their HYDRUS license, i.e., installation, de-installation, and/or reinstallation of HYDRUS. The HYDRUS software package is activated using the **HYDRUS Authorization Status** dialog window (Fig. 153) that is called using the command *Help->Hydrus License and Activation*.

9.2.1. *Brief Description of HYDRUS Activation*

A. **On-Line Activation** (recommended)

- To activate online you need to know your **License Number** (four digits) and the **Activation Key** (hexadecimal, 32 characters). You should receive both numbers from the HYDRUS distributor, from whom you purchased the license for HYDRUS or from HYDRUS customer support support@pc-progress.cz.
- Enter both numbers into the **Online Activation** dialogue window (Fig. 157).
- After clicking the **Activate Now** command, HYDRUS establishes a connection over the Internet with the license server and performs its activation.

B. **Activation by E-Mail** (when encountering problems with on-line activation)
The activation process by email consists of generating two request codes that need to be sent to the HYDRUS distributor together with information about the license, customer, and workplace. Based on this information, the HYDRUS distributor will generate a corresponding activation code and send them back to the HYDRUS user. Different HYDRUS functions will be activated after inserting the activation code depending upon the type of purchased license.

- In the dialog window **Activation by E-mail** (Fig. 171) generate **Request Codes.**
- Send the **Request Codes** by email to support@pc-progress.cz or to the HYDRUS distributor, from whom you purchased the license for HYDRUS.
- After that you will receive by email the **Activation Code**, which you enter into the dialog window **Activation by E-mail** (the **Step 3** Tab, Fig. 163), and activate HYDRUS.

9.2.2. *Detailed Description of HYDRUS Activation*

The **HYDRUS Authorization Status** dialog window (Fig. 153) displays information about **Authorization Status**, **Last Activation**, and **License Information**, such as **License Number**, **Computer ID**, **Workplace**, and **License Owner**. **Authorization Status** information includes information about

a) **Status**, which can be either *Not Authorized* or *Authorization OK*,
b) **Level** of authorization, which can be either *2D-Lite*, *2D-Standard*, *3D-Lite*, *3D-Standard*, or *3D-Professional*,
c) whether or not the **Authorization is Time-Limited** (if yes, then the *Expiration Time* is given), and

d) whether or not the **Network Installation** is active (if yes, then the *Number of Clients* is given)

All this information is displayed as read-only text that is filled in during the first activation of the software. The button "**Send Authorization Report**" is used when resolving problems with software activation.

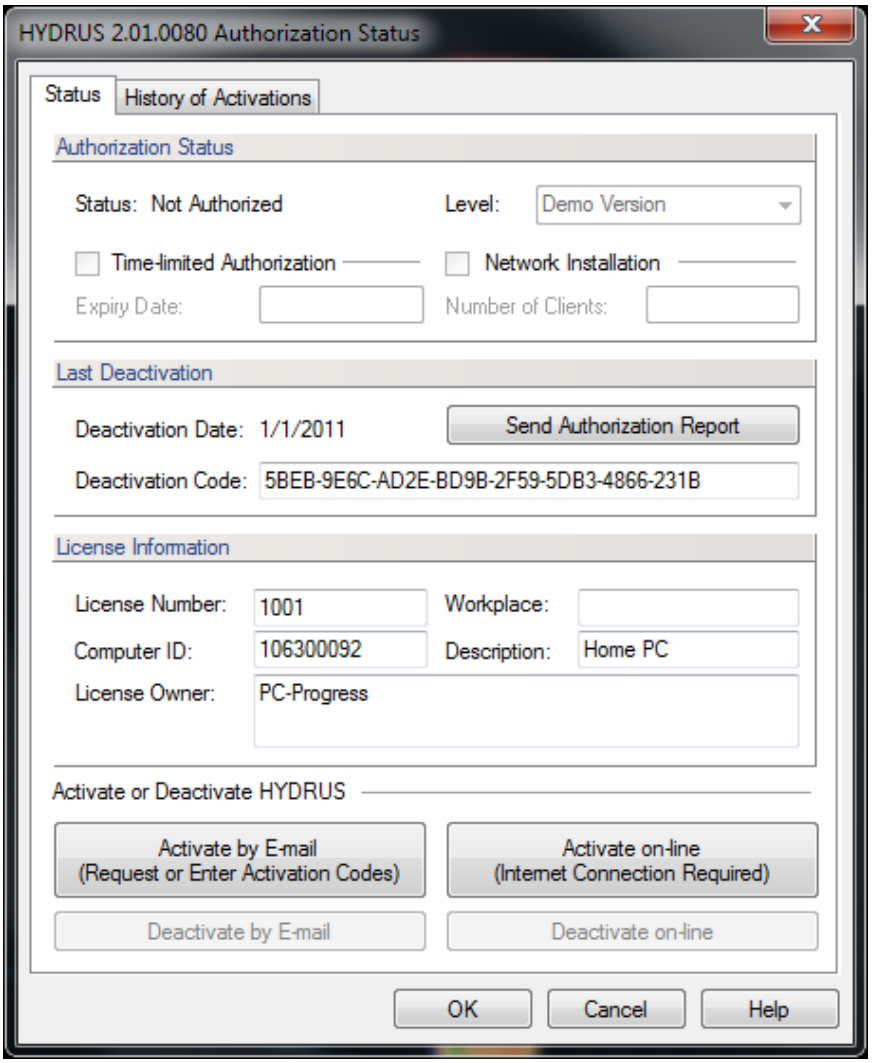


Figure 153. The HYDRUS Authorization Status dialog window (Tab Status).

For the commands in this dialog window to be active (e.g., **Activate by E-mail** or **Activate on-line**), HYDRUS needs to be run with administrator privileges. That means, that you need to be logged as an **Administrator** (or as a user belonging to "Administrators" group) when making changes to the authorization. To run HYDRUS as administrator under Windows Vista or Windows 7 operating systems, click on the HYDRUS icon on your desktop using the right mouse button and select "**Run as Administrator**" from the popup menu. Warning displayed in Figure 154 is issued when attempting to make changes to the **Authorization Status** while not running HYDRUS with administrator privileges.

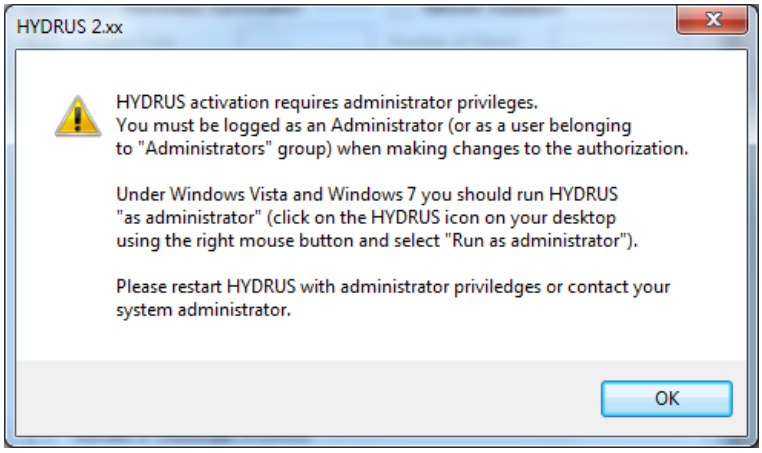

HYDRUS 2.xx
HYDRUS activation requires administrator privileges.
You must be logged as an Administrator (or as a user belonging
to "Administrators" group) when making changes to the authorization.
Under Windows Vista and Windows 7 you should run HYDRUS
"as administrator" (click on the HYDRUS icon on your desktop
using the right mouse button and select "Run as administrator").
Please restart HYDRUS with administrator priviledges or contact your
system administrator.
OK

Figure 154. Warning issued when attempting to make changes to the Authorization Status while not running HYDRUS with administrator privileges.

The second Tab of the **HYDRUS Authorization Status** window, i.e., the **Add-in Modules** Tab list additional HYDRUS modules (e.g., Unsatchem or Wetland) that are currently available and activated.

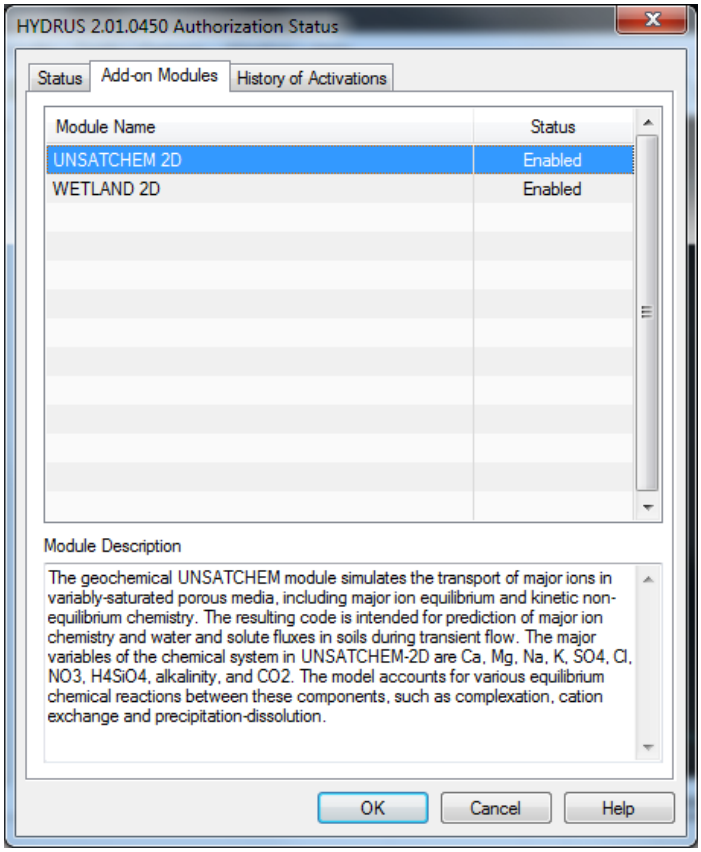

HYDRUS 2.01.0450 Authorization Status
Status
Add-on Modules
History of Activations
Module Name
Status
UNSATCHEM 2D
Enabled
WETLAND 2D
Enabled
Module Description
The geochemical UNSATCHEM module simulates the transport of major ions in variably-saturated porous media, including major ion equilibrium and kinetic non-equilibrium chemistry. The resulting code is intended for prediction of major ion chemistry and water and solute fluxes in soils during transient flow. The major variables of the chemical system in UNSATCHEM-2D are Ca, Mg, Na, K, SO4, Cl, NO3, H4SiO4, alkalinity, and CO2. The model accounts for various equilibrium chemical reactions between these components, such as complexation, cation exchange and precipitation-dissolution.
OK
Cancel
Help

Figure 155. The HYDRUS Authorization Status dialog window (Tab Add-on Modules).

The third Tab of the **HYDRUS Authorization Status** window, i.e., the **History of Activation** Tab reports recent actions related to HYDRUS activation.

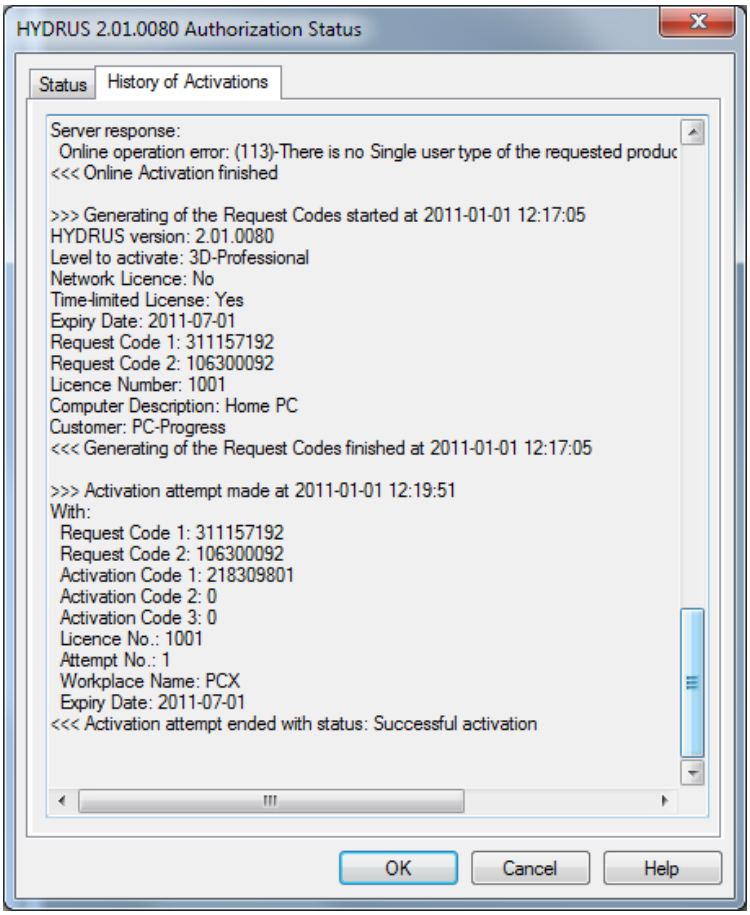


Figure 156. The HYDRUS Authorization Status dialog window (Tab History of Activation).

9.2.2.1. *On-Line Activation*

Online activation is the fastest and most convenient way to activate HYDRUS. The **Online Activation** window (Fig. 157) appears after clicking on the **Activate on-line** button on the **HYDRUS Activation Status** window. Here you need to enter information about the **License Number** and the appropriate **Activation Key** that you received together with an invoice from the HYDRUS Customer Support. This **Activation Key** is used for all Workplaces of a particular license. For special purposes, different **Activation Keys** can be generated for individual Workplaces (e.g., when a particular Workplace has an authorization for a different HYDRUS Level or a specific HYDRUS module).

In the section **Specify the required authorization level** select the required **HYDRUS Level to Activate** (i.e., *2D-Lite*, *2D-Standard*, *3D-Lite*, *3D-Standard*, or *3D-Professional*; please note that this Level has to correspond with the purchased Level) and the Type of License to activate (e.g.,

Time-Limited Authorization with the *Expiration Date*, or the **Network Installation** with the *Number of Clients*). If no checkbox is selected, a **Time-Unlimited Single User License** is authorized. With regard to a possible loss of authorization due to failure of hardware, it is recommended to choose a shorter period of validity (default is 0.5 years). An item **Computer Description** serves for the future identification of a particular computer in the electronic licensing system and is usually characterized by a user or its location (e.g., John - Laptop, Harry - Lab 001).

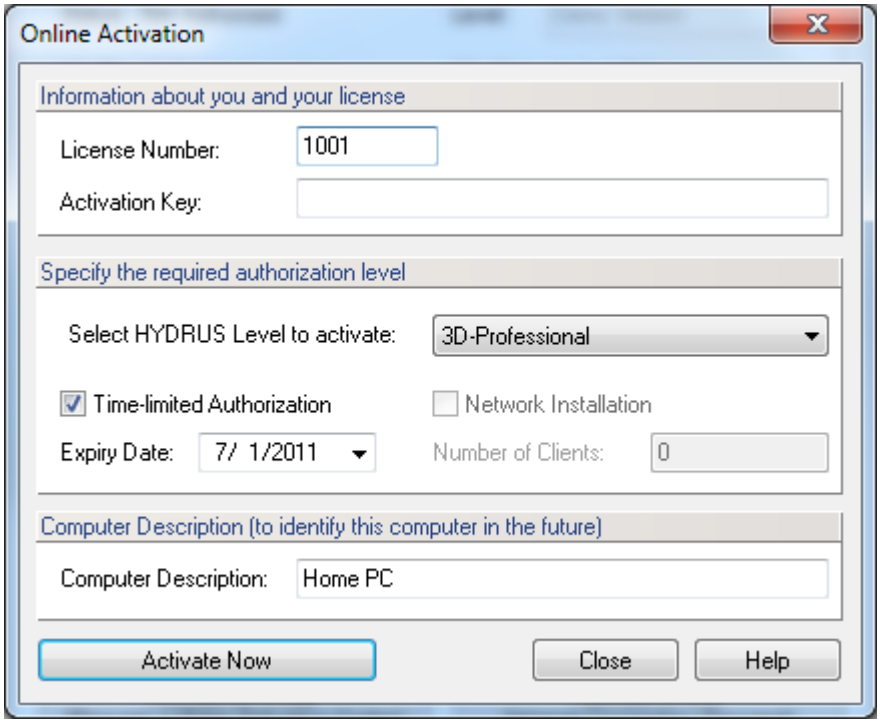


Figure 157. The Online Activation dialog window.

After clicking on the **Activate Now** button, you will be asked to confirm all specified parameters (Fig. 158) (note that you may be prompted by your firewall to allow communication between your computer and the license server of PC Progress). At this point, all specified information will be verified against the data of our electronic licensing system and if confirmed the actual activation of HYDRUS will occur. This communication applies only to data entered in the **Online Activation** window, and no other information stored on your PC is transferred. In case of unsuccessful activation, an error message is displayed explaining the problem. After correcting the problem, you can use again the **Activate Now** command.

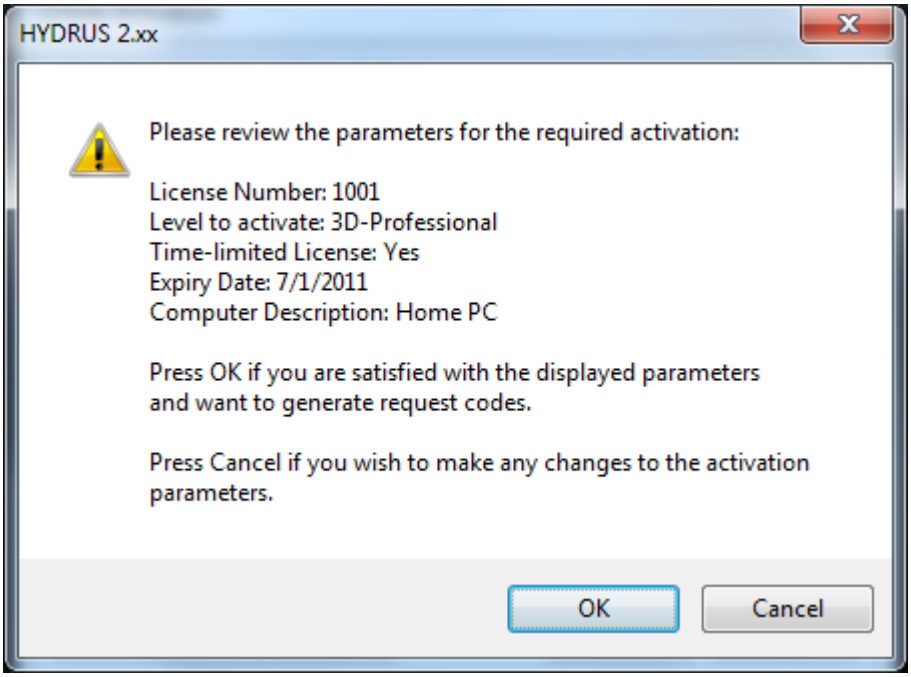

HYDRUS 2.xx
Please review the parameters for the required activation:
License Number: 1001
Level to activate: 3D-Professional
Time-limited License: Yes
Expiry Date: 7/1/2011
Computer Description: Home PC
Press OK if you are satisfied with the displayed parameters and want to generate request codes.
Press Cancel if you wish to make any changes to the activation parameters.
OK
Cancel

Figure 158. Window requesting confirmation of entered parameters.

Prior to the expiration (**Expiry Day**) of the **Time-Limited Authorization**, user will be alerted about it, and the license can be easily repeatedly extended using the **Extend Activation** function.

9.2.2.2. *Activation by E-mail*

For this option, the user is guided through a three-step form (three Tabs of the **Activation by E-mail** dialog window, Fig. 171). During the first two steps he/she prepares information needed to obtain HYDRUS Authorization and emails it to the HYDRUS distributor. In the third step, user enters the **Activation Code** that he receives by e-mail on the third Tab (**Step 3**) of the **Activation by E-mail** and activates HYDRUS.

The first step is to fill in information about the license (**License Number**), the name of the license owner (**Customer**), and description of the Workspace (**WP Description**). This last item (i.e., **WP Description**) serves for future identification of a particular computer in the electronic licensing system and is usually characterized by a user or its location (e.g., John - Laptop, Harry - Lab 001).

In the section **Required Authorization** select the required **HYDRUS Level to Activate** (i.e., *2D-Lite*, *2D-Standard*, *3D-Lite*, *3D-Standard*, or *3D-Professional*; please note that this Level has to correspond with the purchased Level) and the Type of License to activate (e.g., **Time-Limited Authorization** with the *Expiration Date*, or the **Network Installation** with the *Number of Clients*). If no checkbox is selected, a **Time-Unlimited Single User License** is authorized. With regard to a possible loss of authorization due to failure of hardware, it is recommended to choose a shorter period of validity (default is 0.5 years).

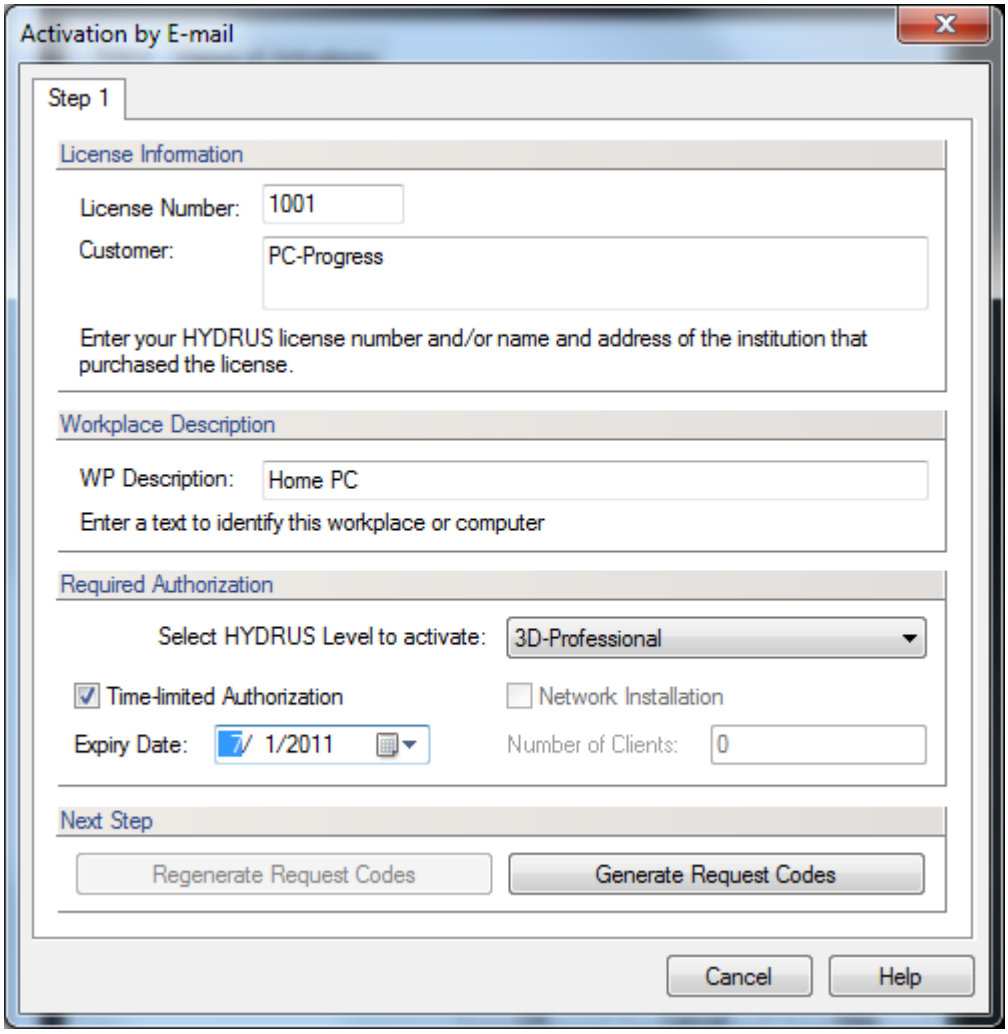


Figure 159. The Activation by E-mail dialog window (Tab Step 1).

After clicking on the **Generate Request Codes** button on Tab **Step 1** of the **Activation by E-mail** window (Fig. 171), user is prompted to confirm all entered information (Fig. 158) and then the Tab **Step 2** (Fig. 160) appears.

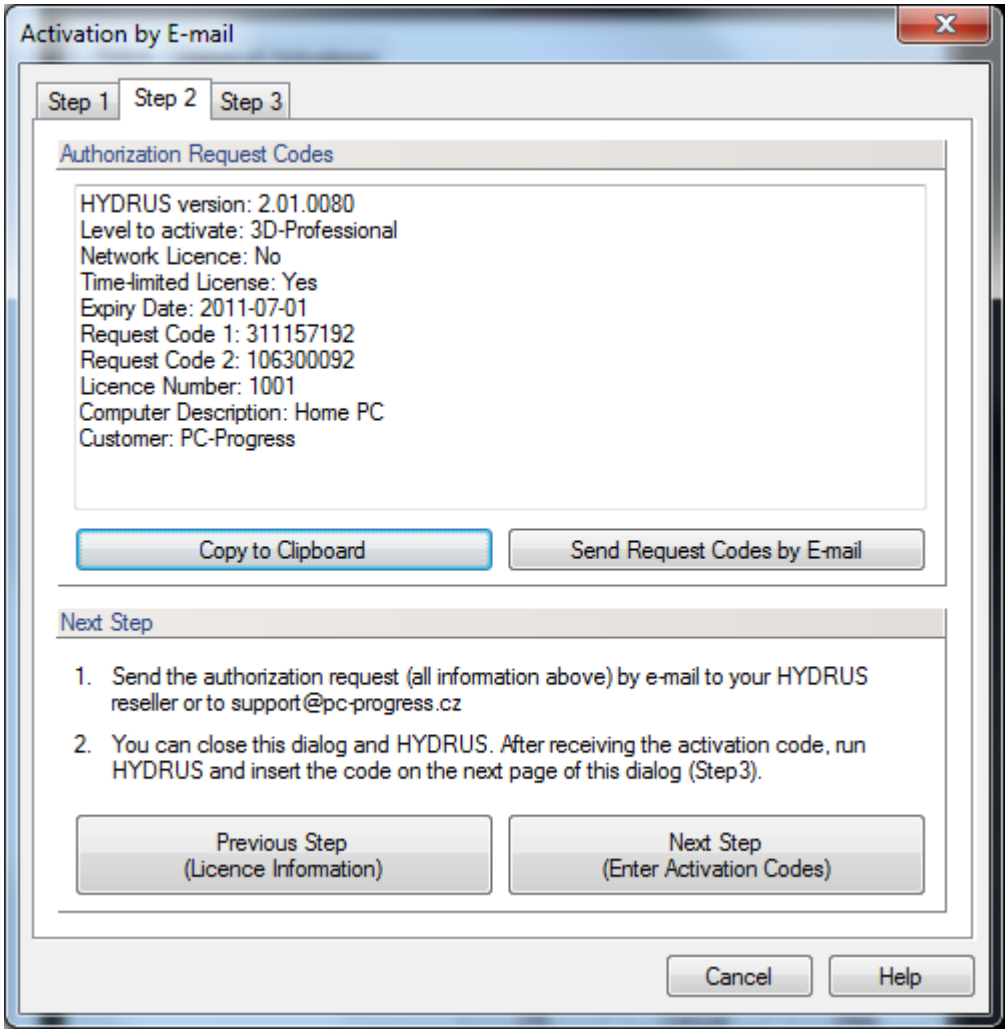

Activation by E-mail
Step 1
Step 2
Step 3
Authorization Request Codes
HYDRUS version: 2.01.0080
Level to activate: 3D-Professional
Network Licence: No
Time-limited License: Yes
Expiry Date: 2011-07-01
Request Code 1: 311157192
Request Code 2: 106300092
Licence Number: 1001
Computer Description: Home PC
Customer: PC-Progress
Copy to Clipboard
Send Request Codes by E-mail
Next Step
1. Send the authorization request (all information above) by e-mail to your HYDRUS reseller or to support@pc-progress.cz
2. You can close this dialog and HYDRUS. After receiving the activation code, run HYDRUS and insert the code on the next page of this dialog (Step3).
Previous Step (Licence Information)
Next Step (Enter Activation Codes)
Cancel
Help

Figure 160. The Activation by E-mail dialog window (Tab Step 2).

Information entered during **Step** 1 (on Tab Step 1) is summarized in the **Authorization Request Codes** section of the **Step 2** Tab. This information can be copied to the clipboard using the **Copy to Clipboard** button and then sent by email to the HYDRUS support or other HYDRUS distributors. The command **Send Request Codes by E-mail** will attempt to start emailing program (e.g., Microsoft Outlook) directly and copy there automatically an email address of the HYDRUS support (support@pc-progress.cz) and all required information (see an example of such email displayed in Outlook in Fig. 161).

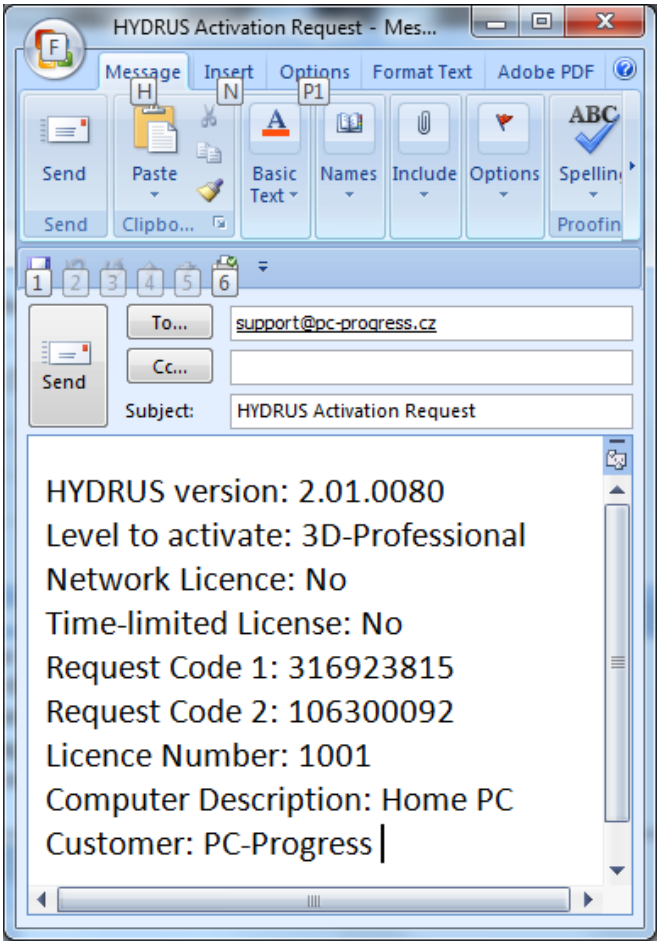


Figure 161. Email with the HYDRUS Activation Request in Outlook.

On the basis of this information, the HYDRUS support or other resellers will promptly email back the **Activation Code**.

Notes on Request Codes

1. Request Code 1 is a randomly generated number that can be used for a single activation. After the activation (either successful or unsuccessful), this number is changed and therefore the same number cannot be used repeatedly even for the same computer.
2. Request Code 2 (Computer ID) is a number that uniquely characterizes the hardware of a computer or a computer network (for the network license). This number should be constant for a particular computer, unless there is a change of hardware. If this number changes, the authorization system will evaluate the license as invalid. It is thus necessary before the change of hardware (e.g., a change of the motherboard) or reinstallation of the operational system (Windows) to deactivate HYDRUS, since HYDRUS will need to be reactivated after hardware changes are completed.
3. There are only three attempts available to activate HYDRUS with particular request and activation codes. If wrong activation codes are inserted during the first three attempts,

HYDRUS issues a warning. After the third attempt with wrong activation codes, the Request Code 1 is changed and new activation codes need to be requested.

4. We recommend using standard functions Copy & Paste when inserting activation codes to minimize risk of inserting wrong numbers.

When starting unauthorized HYDRUS again, user is informed that request codes have recently been generated and if he/she wants to enter the **Activation Code** and activate HYDRUS (Fig. 162). It is important not to regenerate request codes at this time as the **Activation Code** would then not be active any more, since one of the request codes would be changed.

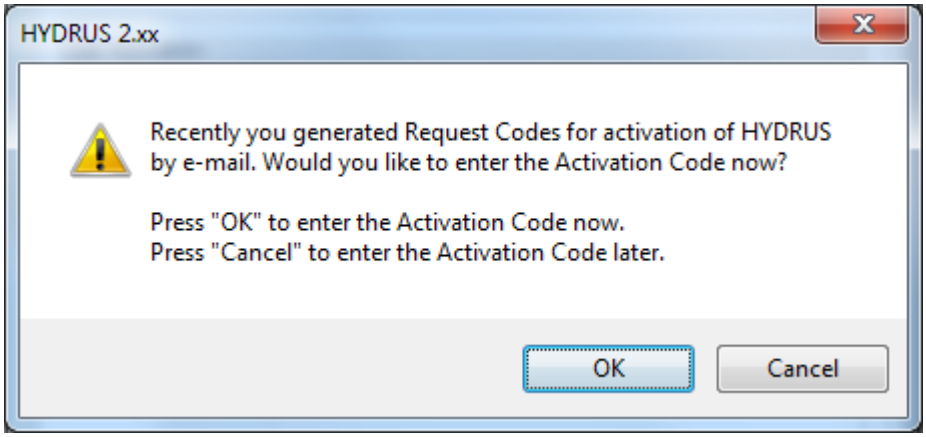

HYDRUS 2.xx
Recently you generated Request Codes for activation of HYDRUS by e-mail. Would you like to enter the Activation Code now?
Press "OK" to enter the Activation Code now.
Press "Cancel" to enter the Activation Code later.
OK
Cancel

Figure 162. Window inquiring if the user wants to enter the Activation Code.

After receiving the **Activation Code**, enter this code on the **Step 3** Tab of the **Activation by E-mail** dialog window (Fig. 163) and click on the **Activate Now** button. You should receive a confirmation that the authorization process was successful (Fig. 164).

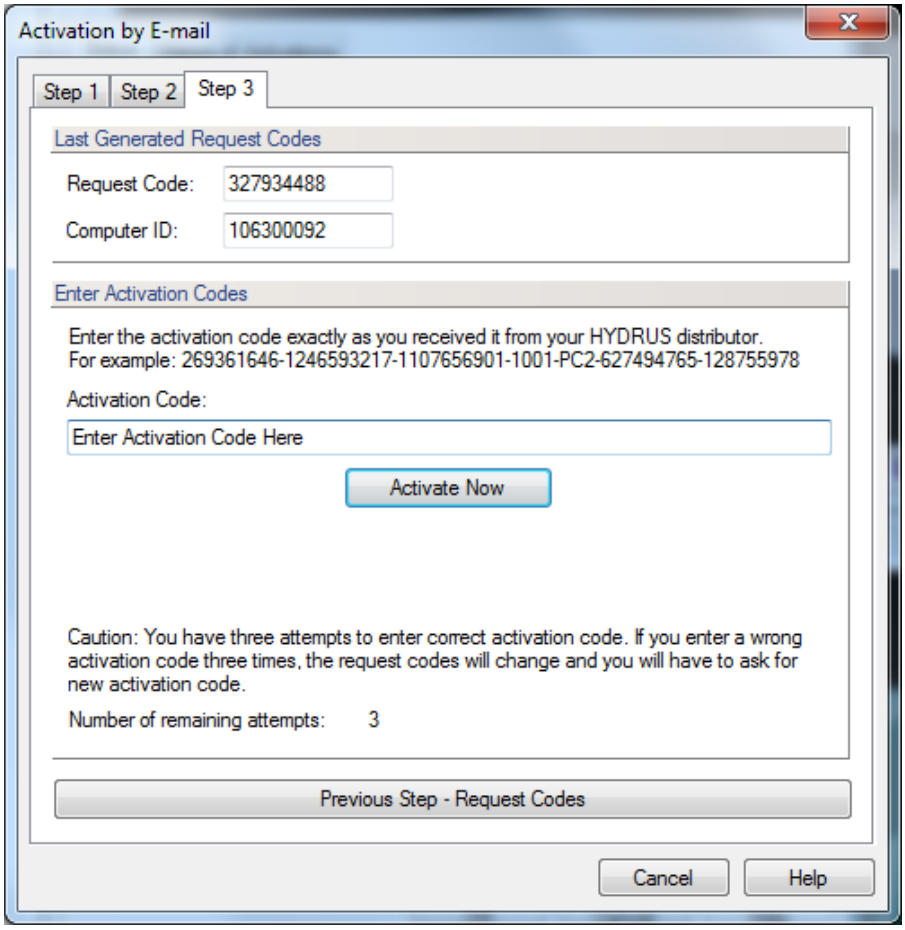

Activation by E-mail
Step 1
Step 2
Step 3
Last Generated Request Codes
Request Code:
327934488
Computer ID:
106300092
Enter Activation Codes
Enter the activation code exactly as you received it from your HYDRUS distributor.
For example: 269361646-1246593217-1107656901-1001-PC2-627494765-128755978
Activation Code:
Enter Activation Code Here
Activate Now
Caution: You have three attempts to enter correct activation code. If you enter a wrong activation code three times, the request codes will change and you will have to ask for new activation code.
Number of remaining attempts:
3
Previous Step - Request Codes
Cancel
Help

Figure 163. The Activation by E-mail dialog window (Tab Step 3).

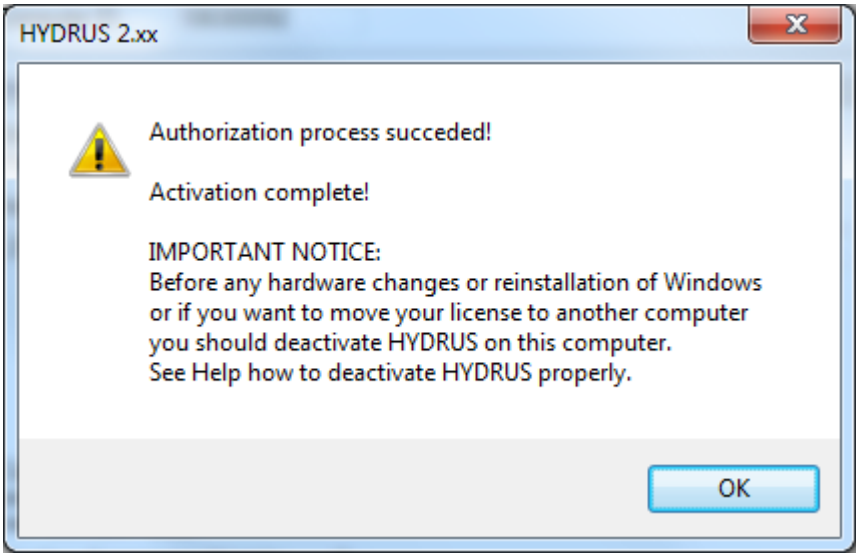

HYDRUS 2.xx
Authorization process succeded!
Activation complete!
IMPORTANT NOTICE:
Before any hardware changes or reinstallation of Windows or if you want to move your license to another computer you should deactivate HYDRUS on this computer.
See Help how to deactivate HYDRUS properly.
OK

Figure 164. Window confirming successful HYDRUS authorization.

Note that the **Request Code** and a **Computer ID** are displayed in the upper part of the **Step 3** Tab. Remember that your Request Code and Computer ID are hardware-dependent. After upgrading your hardware (e.g., BIOS, hard drives), you will very likely have to request new **Activation Code**. You are eligible to obtain those codes for free (although subject to some limitations - ask for details).

When the activation fails three times (likely due to incorrectly entered information), the request keys will change and windows shown in Figure 165 will be displayed, providing instructions on how to proceed further. User will be requested to send a report to the HYDRUS support, so that the cause of the problem can be analyzed.

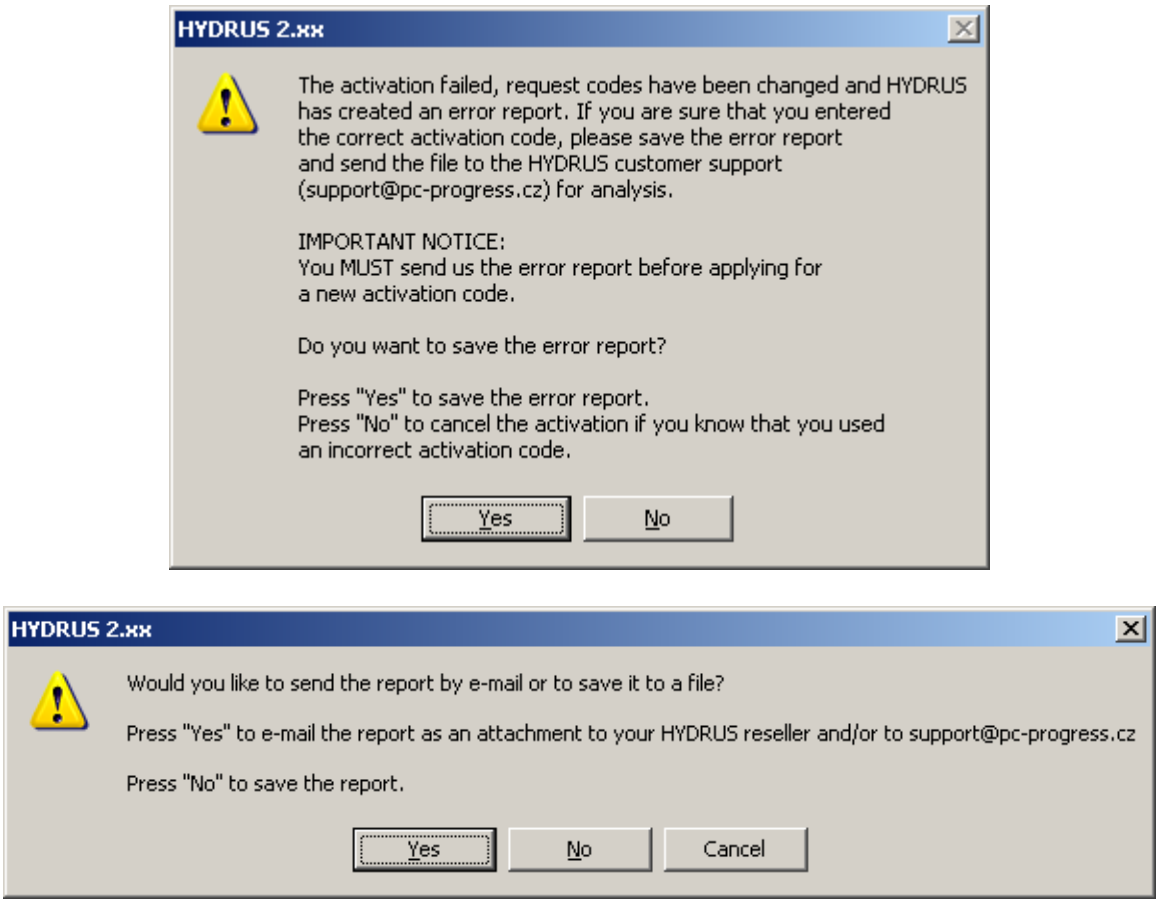

HYDRUS 2.xx
The activation failed, request codes have been changed and HYDRUS has created an error report. If you are sure that you entered the correct activation code, please save the error report and send the file to the HYDRUS customer support (support@pc-progress.cz) for analysis.
IMPORTANT NOTICE:
You MUST send us the error report before applying for a new activation code.
Do you want to save the error report?
Press "Yes" to save the error report.
Press "No" to cancel the activation if you know that you used an incorrect activation code.
Yes
No
HYDRUS 2.xx
Would you like to send the report by e-mail or to save it to a file?
Press "Yes" to e-mail the report as an attachment to your HYDRUS reseller and/or to support@pc-progress.cz
Press "No" to save the report.
Yes
No
Cancel

Figure 165. Window reporting a failure of HYDRUS authorization.

9.2.3. *Reinstallation, Moving to another Computer*

With a "single user" license you are eligible to install and use HYDRUS on two computers (for example a computer in your office and your notebook). If you reinstall HYDRUS on an activated computer or if you install a newer HYDRUS version then your previous authorization will remain active.

Deactivation of HYDRUS and/or Reinstallation to another computer

Users should deactivate HYDRUS before a) any hardware change (motherboard, hard-drives, graphic card, BIOS, etc), b) reinstallation of the Windows OS, c) reformatting the hard-drive with HYDRUS, d) changing the network path to HYDRUS (applies to the network installation), and e) moving HYDRUS license to another computer. The HYDRUS software package is deactivated using the **HYDRUS Authorization Status** dialog window (Fig. 153) that is called using the command *Help->Hydrus License and Activation*. Similarly as for HYDRUS activation, you can deactivate HYDRUS either by email (the command *Deactivate by E-mail*) or online (the command *Deactivate on-line*).

9.2.3.1. *On-Line Deactivation*

After clicking on the command *Deactivate on-line* in the **HYDRUS Authorization Status** dialog window (Fig. 153), in the **Online Deactivation** window (Fig. 166) enter the **Activation Key** and press the button **Deactivate Now**. You should receive a warning that this action will deactivate HYDRUS, and after clicking Yes the confirmation that HYDRUS has been successfully deactivated on your computer (Fig. 167).

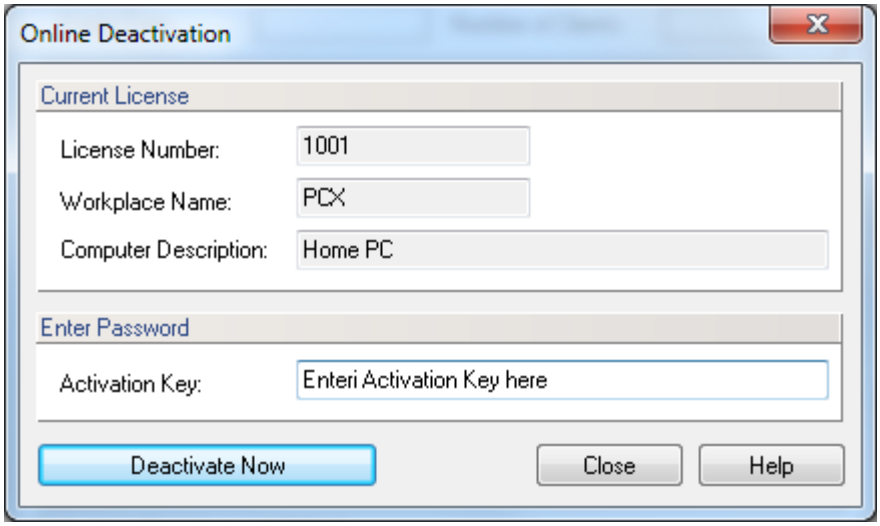


Figure 166. The Online Deactivation dialog window.

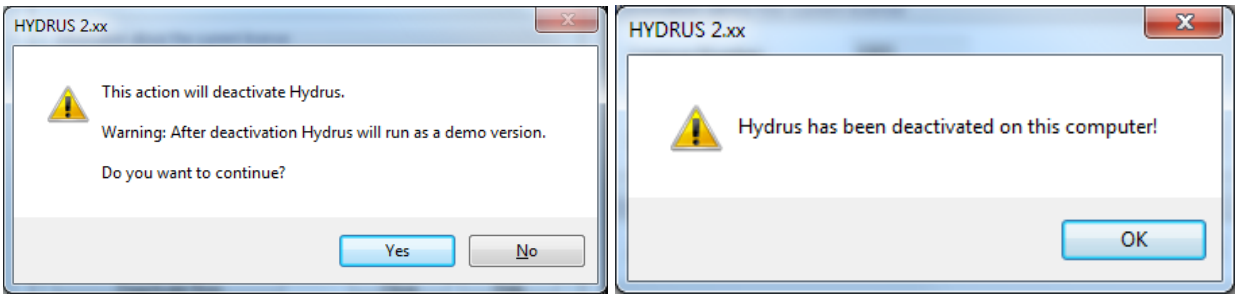


Figure 167. Window confirming successful online deactivation of HYDRUS.

9.2.3.2. *Deactivation by Email*

After clicking on the command *Deactivate by E-mail* in the **HYDRUS Authorization Status** dialog window (Fig. 153), in the **HYDRUS Deactivation** window (Fig. 168) press the button **Deactivate HYDRUS Now**. You should receive a series of warnings that this action will deactivate HYDRUS, and after clicking Yes the confirmation that HYDRUS has been successfully deactivated on your computer (Fig. 169). The **Deactivation Code** will then appear in the **HYDRUS Deactivation** window (Fig. 168). This code can be copied to the clipboard using the **Copy to Clipboard** button and then sent by email to the HYDRUS support or other HYDRUS distributors. The command **Send Deactivation Code by E-mail** will attempt to start emailing program (e.g., Microsoft Outlook) directly and copy there automatically an email address of the HYDRUS support (support@pc-progress.cz) and all required information (see an example of such email displayed in Outlook in Fig. 161).

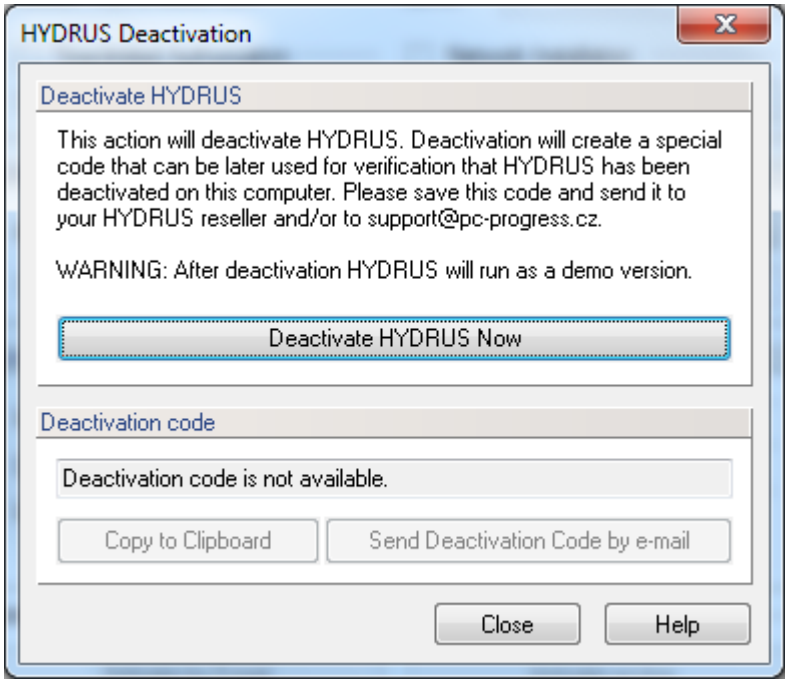

HYDRUS Deactivation
Deactivate HYDRUS
This action will deactivate HYDRUS. Deactivation will create a special code that can be later used for verification that HYDRUS has been deactivated on this computer. Please save this code and send it to your HYDRUS reseller and/or to support@pc-progress.cz.
WARNING: After deactivation HYDRUS will run as a demo version.
Deactivate HYDRUS Now
Deactivation code
Deactivation code is not available.
Copy to Clipboard
Send Deactivation Code by e-mail
Close
Help

Figure 168. The HYDRUS Deactivation dialog window.

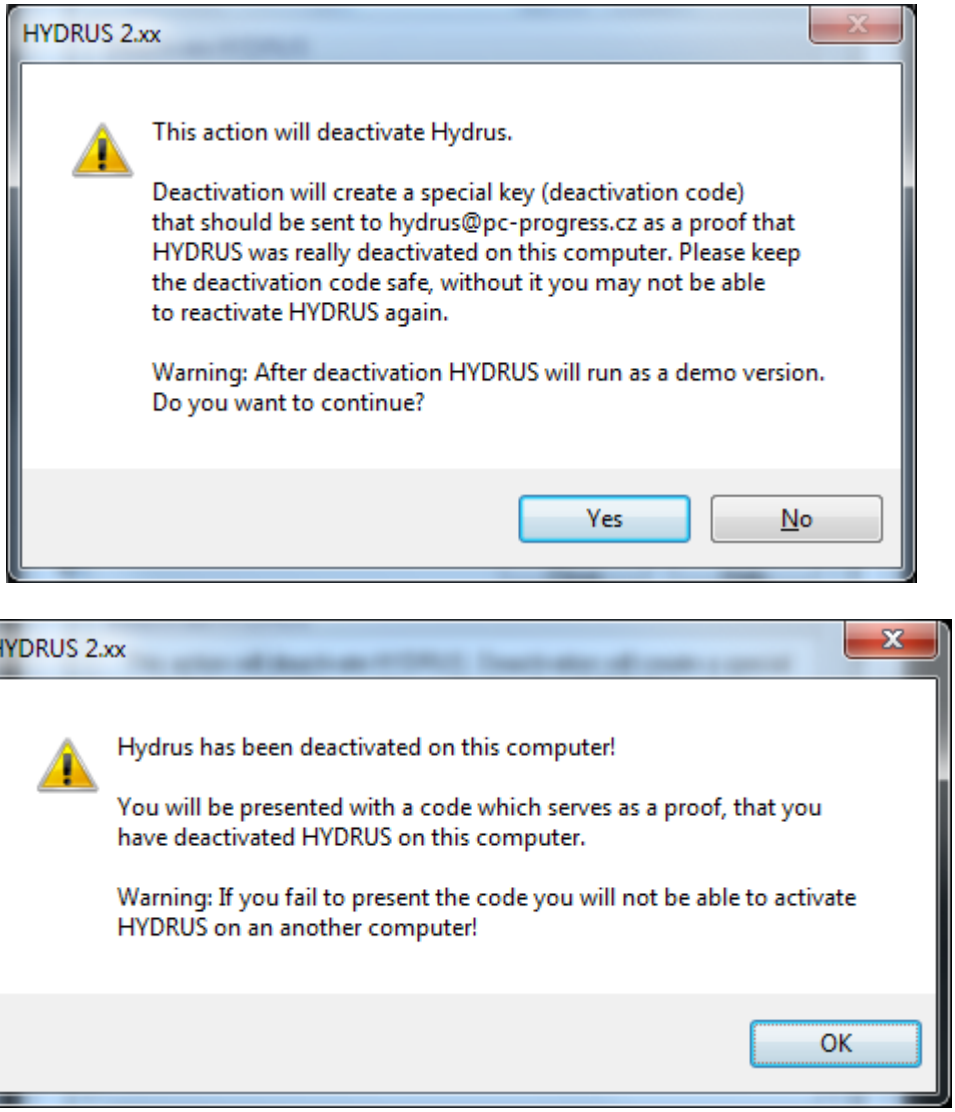

HYDRUS 2.xx
This action will deactivate Hydrus.
Deactivation will create a special key (deactivation code) that should be sent to hydrus@pc-progress.cz as a proof that HYDRUS was really deactivated on this computer. Please keep the deactivation code safe, without it you may not be able to reactivate HYDRUS again.
Warning: After deactivation HYDRUS will run as a demo version. Do you want to continue?
Yes
No
HYDRUS 2.xx
Hydrus has been deactivated on this computer!
You will be presented with a code which serves as a proof, that you have deactivated HYDRUS on this computer.
Warning: If you fail to present the code you will not be able to activate HYDRUS on an another computer!
OK

Figure 169. Window confirming successful deactivation of HYDRUS by email.

9.2.4. *Extending Activation*

Prior to the expiration (**Expiry Day**) of the **Time-Limited Authorization**, user will be alerted about it, and the license can be easily repeatedly extended using the **Extend Activation On-Line** button. This button will appear instead of the **Activate on-line** button on the **Status** Tab of the **HYDRUS Authorization Status** window (Fig. 153). To extend the activation, you will need again the **Activation Key** (either for the entire license or for a particular Workspace).

9.3. *Print Options Dialog Window*

The **Print Options** dialog window contains three tabs (Fig. 170). In the **General Tab** a user selects whether the content of the View window (*Picture*) is to be printed with or without a **Legend**, **Page Orientation** (Portrait or Landscape), and **Page Margins**. In the **Picture Tab**, users further select **Print Quality** (the Standard print quality, which can be changed by users, is 5,000*5,000 pixels), whether the **Frame** is to be printed in black or color (**Colors and Frame**), and **Text Size**. Finally, in the **Legend Tab**, users select what texts **(Legend Rows)** are to be printed, with what **Font**, and how far from the picture. Users can use a predefined text or can write their own.

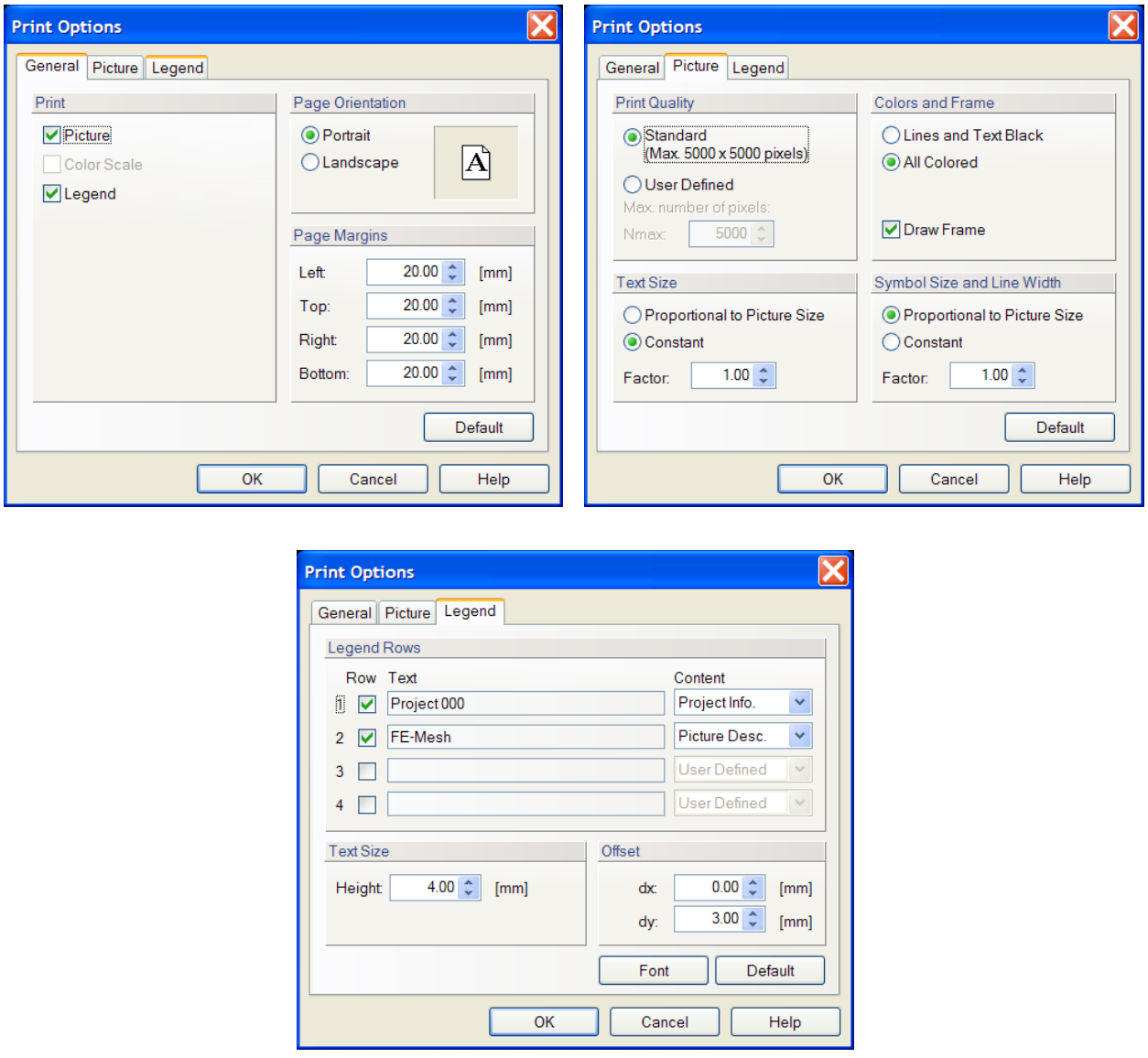


Figure 170. The General, Picture, and Legend tabs of the Print Options dialog window.

9.4. *Print Preview and Copy to the Clipboard Commands*

Result of commands **Print Preview** and **Copy to the Clipboard** is shown in Figure 171. The **Print Preview** command displays the content of the **View Window** on the screen as it would appear in printed formed, while the **Copy to the Clipboard** command copies the same content to a metafile (enhanced metafile, EMF, http://en.wikipedia.org/wiki/Windows_Metafile) in the Clipboard for subsequent pasting into other software packages, such as Word, PowerPoint, etc. Additional content of the metafile (in addition to the content in the View Window, such as the text of the legend) is defined using the **Print Options** window. The metafile contains the bitmap (the resolution of this bitmap (max 6000x6000 pixels) can be specified in the Print Option window) with the graphics displayed in the View Window and additional vector objects (e.g., texts and/or numbering).

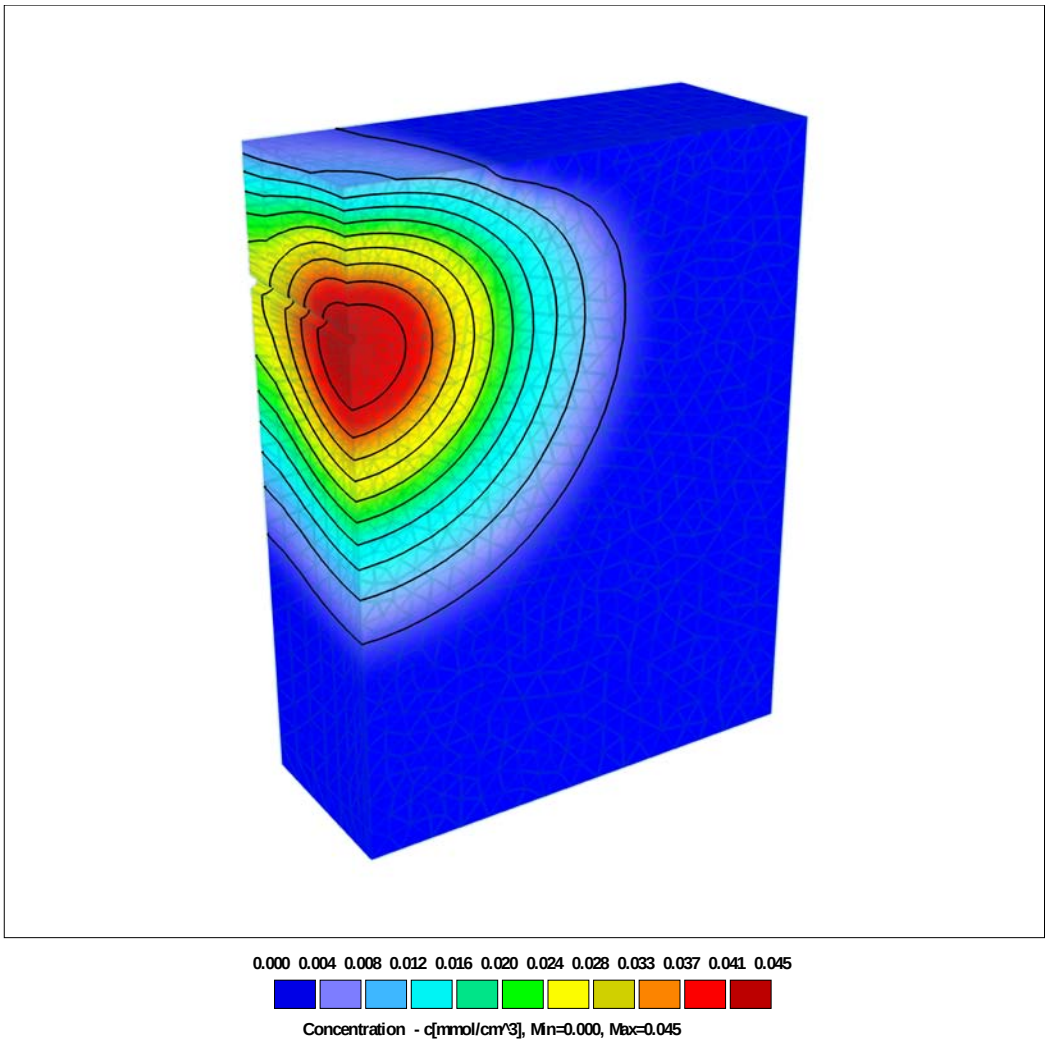

0.000 0.004 0.008 0.012 0.016 0.020 0.024 0.028 0.033 0.037 0.041 0.045
Concentration - c[mmol/cm^3], Min=0.000, Max=0.045
Project 3DFumig6 - 3D, Finite res., Heat Tr., Tarp, Tarp removal, part untarped
Results, Concentration, Time 6 - 1.50 days

Figure 171. Result of commands Print Preview or Copy to the Clipboard.

9.5. *Coordinate systems*

The **Coordinate System** to be used for the transport domain definition can be selected from the **List of Available Coordinate Systems** dialog window (Fig. 172, top) called by the *Tools->Coordinate System* command. **Cartesian**, **Cylindrical**, and **Spherical** systems are available. The **Cartesian** coordinate system is selected by default. A **New Coordinate System** can be defined using the dialog window of the same name (Fig. 172, bottom).

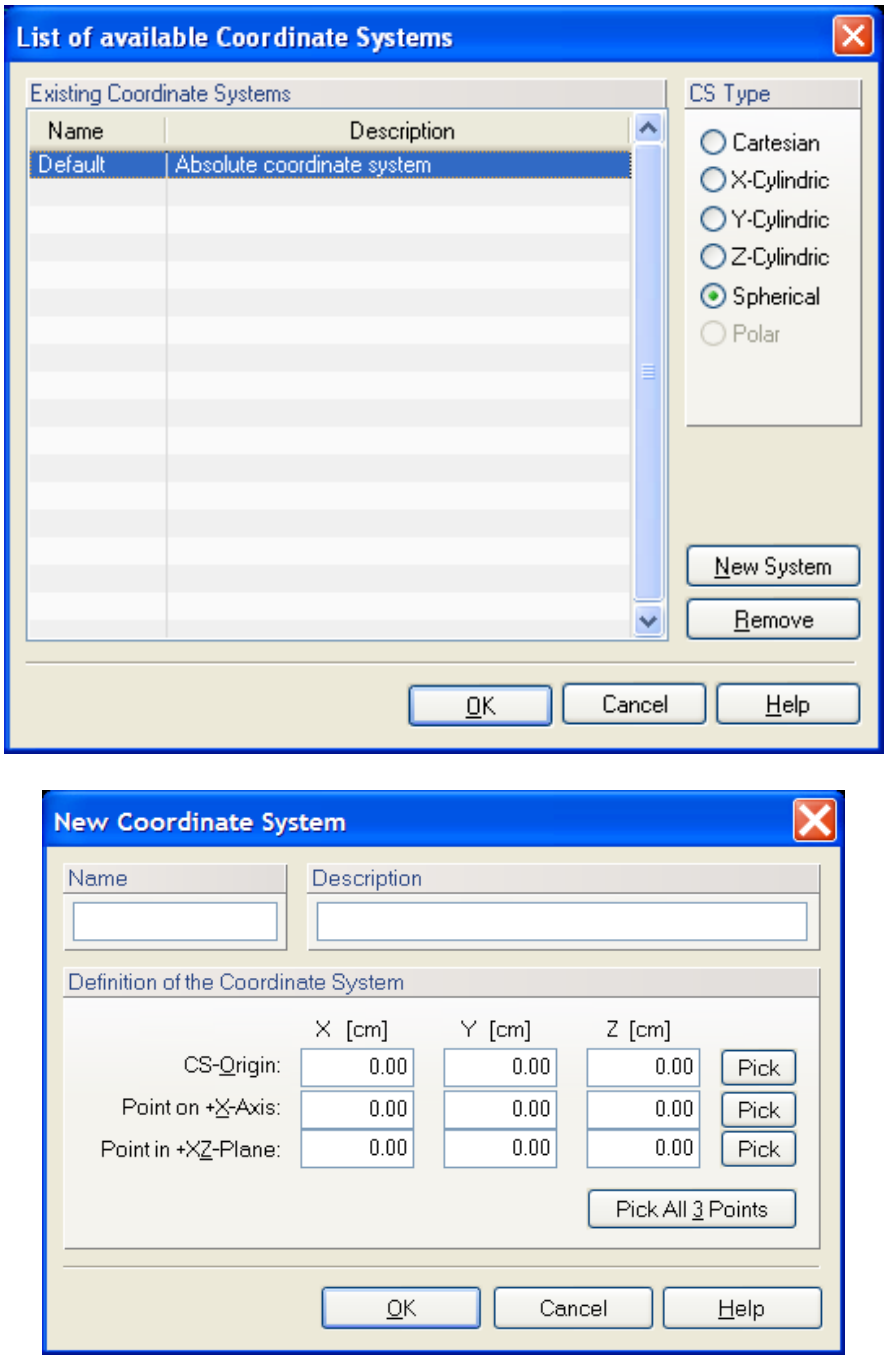


Figure 172. The Coordinate Systems dialog windows.

9.6. *DOS Window During Calculations*

During the calculations different type of information can be written to the screen. The following information may be written to the screen depending upon the problem:

Time	Time
T-Level	Time level
ItW	Number of iterations to solve the water flow problem at a certain time step
ItC	Number of iterations to solve the solute transport problem at a certain time step
ItCum	Cumulative number of iterations
CumAtmBC	Cumulative flux across the atmospheric boundary
CumConst	Cumulative flux across the boundary having a constant flux or pressure head
CumDrain	Cumulative flux across the boundary having a time-variable flux or pressure head
CumRootUp	Cumulative actual root water uptake
CumCh0	Cumulative zero-order production in domain (solute transport)
CumCh1	Cumulative first-order degradation in domain (solute transport)
CumChS	Cumulative solute flux across the boundary having a time-variable flux or pressure head
hAtm	The average pressure head at the atmospheric boundary
hConst	The average pressure head at the boundary having a constant flux or pressure head
hDrain	The average pressure head at the boundary having a time-variable flux or pressure head
hRoot	The average pressure head in the root zone
hSeep	The average pressure head at the boundary with the seepage face
vConstBC	Flux across the boundary having a constant flux or pressure head
vSeep	Flux across the boundary having a seepage face

9.7. *Video Files*

Users can save the flow animation using the **Create Video File** command (Tools->Create Video File). This command calls the **Create Video File** dialog window (Fig. 173), in which a user needs to specify where the *Video File* should be saved and under what name, type of the video file [a) Cinepac Codec by Radius, b) Microsoft Video 1, c) Intel Indeo Video 4.5, d) Intel Indeo Video 5.10, e) Microsoft MPEG-4 Video Codec V1, and f) Microsoft MPEG-4 Video Codec V2] and its *Quality*, and finally whether recording is carried out at *Real Time* (i.e., video will run at the same speed as HYDRUS animation) or only when frames in the View Window change (only changes in View Window are recorded). Additional options (such as Smoothness, Data Rate (i.e., kilobits per second)) are available for each particular video format. OpenGL acceleration should be disabled when problems occur when creating Video File.

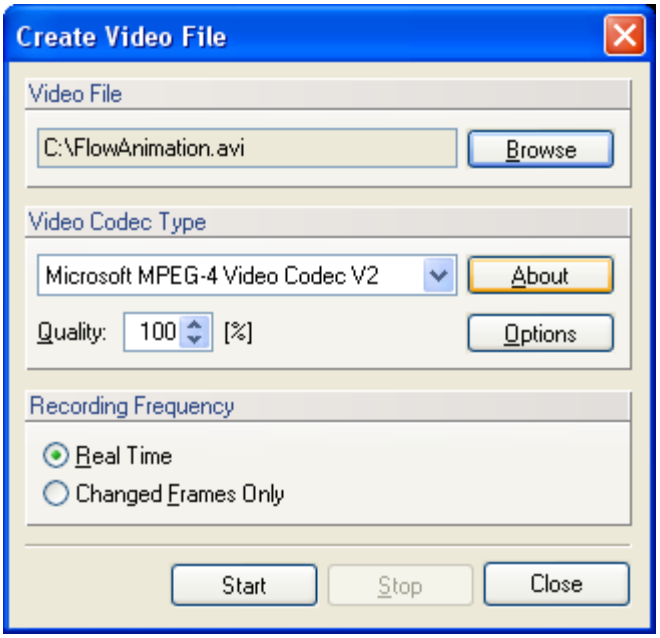


Figure 173. The Create Video File dialog window.

Notes on Video Editing:

1. Video records only changes in View. Thus, if nothing changes in the View window, only the first picture is recorded. When one records animation of flow or transport, then while the View window is redrawn, each change is recorded. Similarly, one could record video for any other manipulation of the View, which requires its redrawing (e.g., rotation of the model).

2. If the option "Real-Time" is on, each recorded View has an assigned time, which elapsed between redrawing of the View window. This means that the video is then played at approximately the same rate as redrawing of the View window.

3. If the option "Changed Frames Only" is on, then changes in the View window are stored regardless of the actual time elapsed in redrawing the View. For example, if some changes in redrawing of view take place quickly, followed by a pause, and again fast changes, in the resulting video, all changes will be played back with a constant time delay. The current version of HYDRUS does not have an option allowing to set a time interval between recorded frames. It is entirely possible that one can edit Video recordings created by HYDRUS using some public domain programs for editing videos. We currently do not have any experience with that and can not make any recommendations.

9.8. *About HYDRUS*

This window displays the program version (the Program Tab), authors of the HYDRUS application (the Authors Tab), and the License agreement (the License Agreement Tab). The Program Tab additionally displays other software products (such as mesh generators) that are used in HYDRUS.

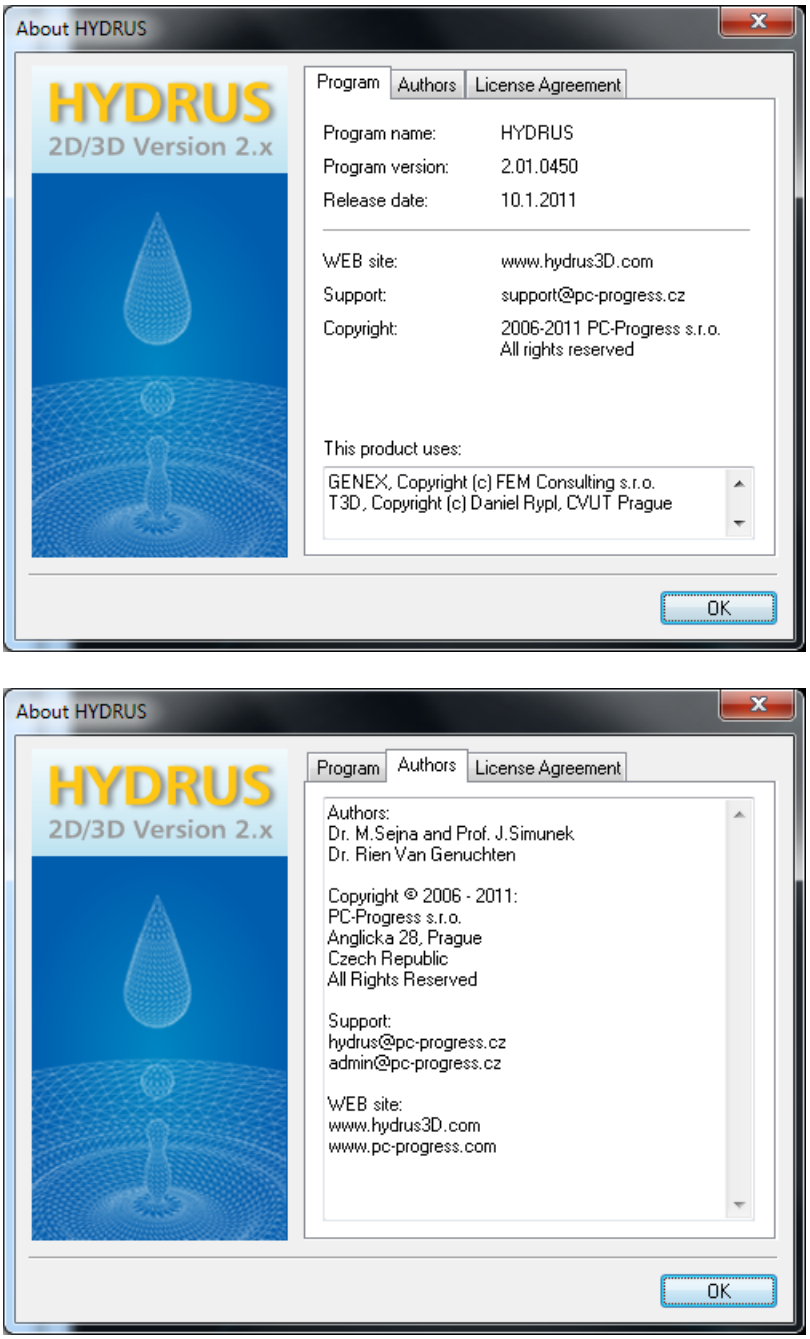


Figure 174. The About HYDRUS dialog window (the Program tab (top) and the Authors tab (bottom).

References

Bradford, S. A., S. R. Yates, M. Bettehar, and J. Šimůnek, Physical factors affecting the transport and fate of colloids in saturated porous media, *Water Resour. Res.,* 38(12), 1327, doi:10.1029/2002WR001340, 63.1-63.12, 2002.

Brooks, R. H., and A. T. Corey, Properties of porous media affecting fluid flow. *J. Irrig. Drainage Div.*, ASCE Proc. 72(IR2), 61-88, 1966.

Carsel, R.F., and Parrish, R. S., Developing joint probability distributions of soil water retention characteristics, *Water Resour. Res, 24,* 755-769, 1988.

Chung S.-O., and R. Horton, Soil heat and water flow with a partial surface mulch, *Water Resour. Res., 23*(12), 2175-2186, 1987.

Durner, W., Hydraulic conductivity estimation for soils with heterogeneous pore structure, *Water Resour. Res*., *32*(9), 211-223, 1994.

Feddes, R. A., P. J. Kowalik, and H. Zaradny, *Simulation of Field Water Use and Crop Yield*, John Wiley & Sons, New York, NY, 1978.

Hopmans, J. W., J. Šimůnek, N. Romano, and W. Durner, Inverse Modeling of Transient Water Flow, In: *Methods of Soil Analysis, Part 1, Physical Methods*, Chapter 3.6.2, Eds. J. H. Dane and G. C. Topp, Third edition, SSSA, Madison, WI, 963-1008, 2002.

Kool, J. B., and J. C. Parker, Development and evaluation of closed-form expressions for hysteretic soil hydraulic properties. *Water Resour. Res., 23*(1), 105-114, 1987.

Kosugi K., Lognormal distribution model for unsaturated soil hydraulic properties, *Water Resour. Res*., *32*(9), 2697-2703, 1996.

Langergraber, G. and J. Šimůnek, Modeling variably-saturated water flow and multi-component reactive transport in constructed wetlands, *Vadose Zone Journal*, *4*, 924-938, 2005.

Langergraber, G., and J. Šimůnek, The Multi-component Reactive Transport Module CW2D for Constructed Wetlands for the HYDRUS Software Package, Manual – Version 1.0, *HYDRUS Software Series 2*, Department of Environmental Sciences, University of California Riverside, Riverside, CA, 72 pp., 2006.

Langergraber, G., D. Rousseau, J. Garcia, and J. Mean, CWM1 - A general model to describe biokinetic processes in subsurface flow constructed wetlands, *Water Science Technology*, 59(9), 1687-1697, 2009.

Langergraber, G., and J. Šimůnek, The HYDRUS Wetlands Module, Version 2, *HYDRUS Software Series 4*, Department of Environmental Sciences, University of California Riverside, Riverside, CA, 56 pp., 2011.

Lazarovitch, N., J. Šimůnek, and U. Shani, System dependent boundary condition for water flow from subsurface source, *Soil Sci. Soc. Am. J., 69*(1), 46-50, 2005.

Lenhard, R. J., J. C. Parker, and J. J. Kaluarachchi, Comparing simulated and experimental hysteretic two-phase transient fluid flow phenomena, *Water Resour. Res., 27*(8), 2113-2124, 1991.

Lenhard, R. J., and J. C. Parker, Modeling multiphase fluid hysteresis and comparing results to laboratory investigations, In M. Th. van Genuchten, F. J. Leij, and L. J. Lund (eds.), Proc. Intl. Workshop on *Indirect Methods for Estimating the Hydraulic Properties of Unsaturated Soils,* University of California, Riverside, CA, pp. 233-248, 1992.

Maas, E. V., Crop salt tolerance. In K. K. Tanji (ed.), "*Agricultural Salinity Assessment and Management*", ASCE Manuals and Reports on Engineering practice, No. 71, NY, 1990.

McNeal, B. L, Prediction of the effect of mixed-salt solutions on soil hydraulic conductivity, *Soil Sci. Soc. Amer. Proc., 32*, 190-193, 1968.

Millington, R. J., and J. M. Quirk, Permeability of porous solids, *Trans. Faraday Soc., 57*, 1200-1207, 1961.

Moldrup, P., T. Olesen, D. E. Rolston, and T. Yamaguchi, Modeling diffusion and reaction in soils: VII. Predicting gas and ion diffusivity in undisturbed and sieved soils, *Soil Sci., 162*(9), 632-640, 1997.

Moldrup, P., T. Olesen, J. Gamst, P. Schjønning, T. Yamaguchi, and D. E. Rolston, Predicting the gas diffusion coefficient in repacked soil: water-induced linear reduction model, *Soil Sci. Soc. Am. J., 64*, 1588-1594, 2000.

Perrochet, P., and D. Berod, Stability of the standard Crank-Nicolson-Galerkin scheme applied to the diffusion-convection equation: some new insights, *Water Resour. Res., 29*(9), 3291-3297, 1993.

Schaap, M. G., Leij, F. J., and van Genuchten, M. Th., Rosetta: a computer program for estimating soil hydraulic parameters with hierarchical pedotransfer functions, *J. of Hydrol.*, 251, 163-176, 2001.

Scott, P. S., G. J. Farquhar, and N. Kouwen, Hysteresis effects on net infiltration, Advances in Infiltration, *Publ. 11-83*, pp.163-170, Am. Soc. Agri. Eng., St. Joseph, MI, 1983.

Šimůnek, J., and D. L. Suarez, Two-dimensional transport model for variably saturated porous media with major ion chemistry, *Water Resour. Res., 30*(4), 1115-1133, 1994.

Šimůnek, J., and J. W. Hopmans, Parameter Optimization and Nonlinear Fitting, In: *Methods of Soil Analysis, Part 1, Physical Methods*, Chapter 1.7, Eds. J. H. Dane and G. C. Topp, Third edition, SSSA, Madison, WI, 139-157, 2002.

Šimůnek, J., D. Jacques, J. W. Hopmans, M. Inoue, M. Flury, and M. Th. van Genuchten, Solute Transport During Variably-Saturated Flow - Inverse Methods, In: *Methods of Soil Analysis, Part 1, Physical Methods*, Chapter 6.6, Eds. J. H. Dane and G. C. Topp, Third edition, SSSA, Madison, WI, 1435-1449, 2002.

Šimůnek, J., N. J. Jarvis, M. Th. van Genuchten, and A. Gärdenäs, Review and comparison of models for describing non-equilibrium and preferential flow and transport in the vadose zone, *Journal of Hydrology*, 272, 14-35, 2003.

Šimůnek, J., M. Šejna, H. Saito, M. Sakai, and M. Th. van Genuchten, The HYDRUS-1D Software Package for Simulating the Movement of Water, Heat, and Multiple Solutes in Variably Saturated Media, Version 4.0, *HYDRUS Software Series 3*, Department of Environmental Sciences, University of California Riverside, Riverside, California, USA, pp. 315, 2008.

Šimůnek, J., M. Th. van Genuchten, and M. Šejna, Development and applications of the HYDRUS and STANMOD software packages, and related codes, *Vadose Zone Journal*, doi:10.2136/VZJ2007.0077, Special Issue "Vadose Zone Modeling", *7*(2), 587-600, 2008.

Šimůnek, J. and J. W. Hopmans, Modeling compensated root water and nutrient uptake, *Ecological Modeling*, doi:10.1016/j.ecolmodel.2008.11.004, *220*(4), 505-521, 2009.

Šimůnek, J., M. Th. van Genuchten, and M. Šejna, The HYDRUS Software Package for Simulating Two- and Three Dimensional Movement of Water, Heat, and Multiple Solutes in Variably-Saturated Media, Version 2.0, Technical Manual, PC Progress, Prague, Czech Republic, 2011.

Skaggs, T. H., P. J. Shouse, and J. A. Poss, Irrigating Forage Crops with Saline Waters. 2. Modeling Root Uptake and Drainage, *Vadose Zone J., 5*, 824-837, 2006.

Stumm, W., and J. J. Morgan, *Aquatic Chemistry: An Introduction Emphasizing Chemical Equilibria in Natural Waters*, John Wiley & Sons, New York, NY, 1981.

Taylor, S. A. and G. M. Ashcroft, *Physical Edaphology*. Freeman and Co., San Francisco, California, p. 434-435, 1972.

van Genuchten, M. Th., A closed-form equation for predicting the hydraulic conductivity of unsaturated soils, *Soil Sci. Soc. Am. J., 44*, 892-898, 1980.

van Genuchten, M. Th., Convective-dispersive transport of solutes involved in sequential first-order decay reactions, *Computers & Geosci., 11*(2), 129-147, 1985.

Vrugt, J. A., J. W. Hopmans, and J. Šimůnek, Calibration of a two-dimensional root water uptake model, *Soil Sci. Soc. Am. J., 65*(4), 1027-1037, 2001.

Vrugt, J.A., M. T. van Wijk, J. W. Hopmans, and J. Šimůnek, One-, two-, and three-dimensional root water uptake functions for transient modeling, *Water Resour. Res., 37*(10), 2457-2470, 2002.

Vogel, T., and M. Císlerová, On the reliability of unsaturated hydraulic conductivity calculated from the moisture retention curve, *Transport in Porous Media, 3*, 1-15, 1988.

Walker, A., A simulation model for prediction of herbicide persistence, J. Environ. Quality, 3(4), 396-401, 1974.

Wesseling, J. G., J. A. Elbers, P. Kabat, and B. J. van den Broek, SWATRE: instructions for input, Internal Note, Winand Staring Centre, Wageningen, the Netherlands, 1991.

Yeh, G. T., and V. S. Tripathi, HYDROGEOCHEM: A coupled model of HYDROlogic transport and GEOCHEMical equilibria in reactive multicomponent systems, *Environs Sci. Div., Publ. No. 3170.*, Oak Ridge National Lab., Oak Ridge, TN, 1990.